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TECHNICAL ABSTRACTS

TIME-RESOLVED EMISSION SPECTROSCOPIC DETERMINATION OF ROTATIONAL TEMPERATURES IN A HYDROGEN RADIOFREQUENCY DISCHARGE

V. Schulz-Von der Gathen, T. Kawetzki and H.F. Dobele, Universitat GH Essen, Institut fur Laser- und Plasmaphysik, 45117 Essen, Germany (Presented at the *52nd Annual Gaseous Electronics Conference*, Held in Norfolk VA, October 1999).

Spectroscopic gas temperature determination in hydrogen plasmas is commonly based on molecular line intensity ratio measurements of the diagonal bands ($\Delta v=0$) of the Fulcher-α system ($d^3\Pi_u \rightarrow a^3\Sigma_g$). We have studied, in contrast to earlier work where only time-averaged intensities were measured, the temporal behavior of the rotational state distribution along the discharge axis of a CCRF plasma source (10-100 W, 10-100 Pa) with a novel intensified CCD camera. This camera is synchronized to the transceiver frequency and allows measurements with time resolution of 3 ns using each radiofrequency cycle. Rotational temperatures inferred on the basis of collisional excitation from the ground state indicate strong variations during one cycle rising from about 400 K by more than, for example, 100 K at high pressures. We conclude that either more elaborate population models have to be applied or a time interval has to be selected by time-resolved spectroscopy where the underlying assumptions are fulfilled to allow the application of this otherwise very convenient diagnostic.

NITROGEN CARS THERMOMETRY WITHIN THE OUTER JACKET OF A METAL HALIDE LAMP

L.R. Brock and H. Adler, Osram Sylvania Inc. (Presented at the *52nd Annual Gaseous Electronics Conference*, Held in Norfolk VA, October 1999).

High resolution coherent anti-Stokes Raman spectroscopy (CARS) was applied to measure axial and radial temperature profiles within the outer jacket of a 360 W metal halide lamp. The CARS technique was chosen for this task because its good spatial resolution, coherent signal beam, nonintrusive nature, and selectivity yields spectra with very high signal to noise ratios despite the high level of background radiation from the running lamp. We use nitrogen CARS thermometry here because the outer jacket is filled with 400 torr of nitrogen at room temperature. Rotationally resolved nitrogen CARS spectra are measured at a number of points within the metal halide lamp. A spectral simulation program is utilized to calculate spectra for gas temperatures between 500 and 1000 K. A comparison between these simulations and the measured rotationally resolved nitrogen CARS spectra allows the temperature at each point in the lamp to be accurately determined. In addition, good agreement was achieved between the measured temperature distribution and predicted axial and radial temperature profiles in the outer jacket of the metal halide lamp.

Spatially Resolved Measurements of O_2 Vibrational Distribution and Rotational Temperature in Laser-Sustained Nonequilibrium Plasmas

R. Leiweke, M. Fernee, I. Adamovich and W. Lempert, The Ohio State University, Department of Mechanical Engineering, Columbus, OH 43210 (Presented at the *52nd Annual Gaseous Electronics Conference*, Held in Norfolk VA, October 1999).

It is well known that the CO laser can be used to initiate and sustain electron production in pure CO (or mixtures of CO with buffers such as argon and/or nitrogen) at low to modest translational temperature. In this paper, we will present new results which quantify the influence of spatial inhomogeneity in the CO pump laser intensity on the vibrational distribution of O_2 in high pressure $N_2/O_2/CO$ and $Ar/O_2/CO$ plasmas. This will be accomplished by Planar Laser Induced Fluorescence (PLIF) using the well-known Schumann-Runge bands of molecular oxygen. The primary objective of the work to be presented is the experimental verification of predictions from detailed 'Master Equation' kinetic modeling codes. Determination of O_2 vibrational populations for $v''=0$-3 will be achieved using an ArF excimer laser at about 193 nm. Levels 4-7 will be measured using KrF at about 248 nm. A secondary objective will be to determine the spatial dependence of the heavy gas translational/rotational temperature, which will be inferred from the rotationally resolved O_2 LIF spectra. Complementary spatially averaged electron density measurements will be performed by determining classical current-voltage characteristics.

Hopping Motion in a Chemically Reacting System

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Heavy hydrocarbon premixed flames form ordered patterns of concentric rings of brighter (hotter) cells separated by darker (cooler) cusps and folds. One of the (four) dynamic states that are unique to this system is a hopping motion in which individual cells in a ring sequentially change their position by abrupt angular displacements. Our analysis based on bifurcations with symmetry shows that hopping states are mixed-mode states that result from an interaction of an N-fold symmetric rotating wave state with an (N-1)-fold symmetric rotating wave state. However, the resulting hopping state is not a traveling wave state because some cells remain fixed while others execute hopping motion. Hopping states have also been described as 'pushmepullyou' states in numerical studies by Bayliss and Matkowsky. Videotaped examples of this dynamics will be shown.

Higher Order Diffusion of the Helium Triplet Metastable Measured by Diode Laser Absorption

M. Millard and P. Yaney, University of Dayton, and B. Ganguly and C.A. DeJoseph Jr, Air Force Research Laboratory, Wright-Patterson AFB, OH (Presented at the *52nd Annual Gaseous Electronics Conference*, Held in Norfolk VA, October 1999).

We have used an InGaAs Bragg-Reflecting Diode Laser to study the diffusion of the 2^3S_1 metastable of helium at 1.083 μm by diode laser absorption. A pulsed parallel-plate discharge with 50 mm diameter electrodes with a spacing of 16 mm was used. A glass sleeve with two 2 mm wide slits for optical access was placed over the electrodes to constrain the discharge to the region between the electrodes and to control the exact geometry of the problem. Data were obtained at 2 and 5 torr using a flow-rate of less than 1 sccm. A measured value of 478(±15) cm^2/s was obtained for the diffusion constant after correcting for temperature and pressure. The data also showed the presence of higher order diffusion modes. Analysis of these modes was performed using a method based on the work of Chantry and by comparison with a 2-dimensional numerical model of the diffusion in the chamber. The results of these analyses and a discussion of the problems imposed by the system will be presented.

Gas Phase Ion-Molecule Reactions in Perfluoropropane

C.Q. Jiao and P.D. Haaland, Mobium Enterprises, Inc., Dayton OH, and C.A. DeJoseph Jr and A. Garscadden, Air Force Research Laboratory, Wright-Patterson AFB, OH (Presented at the *52nd Annual Gaseous Electronics Conference*, Held in Norfolk VA, October 1999).

Ions in the gas phase generated by the electron impact ionization of perfluoropropane (C_3F_8) at 25 and 50 eV, respectively, were studied to measure their reactions with the parent molecule at room temperature in the 10^{-7} torr s range. Among the ions observed, CF_3^+, $C_2F_4^+$ and $C_2F_5^+$ were found to be unreactive (rate constant $<10^{-12}$ cm^3 s^{-1}) with C_3F_8, while CF^+ and CF_2^+ reacted forming mainly $C_3F_7^+$ with rate constants of 1.5(±0.2)10^{-11} and 7.0(±0.5)10^{-11} cm^3 s^{-1}, respectively, and $C_3F_7^+$ reacted to form CF_3^+ and $C_2F_5^+$ with a rate constant of 8.6(±0.5)10^{-11} cm^3 s^{-1}. Ar^+ (formed by electron impact on Ar) has also been studied and found to react with C_3F_8 to yield mainly $C_3F_7^+$ and CF_3^+, with a rate constant of 3.9(±0.4)10^{-10} cm^3 s^{-1}. The reactivity of all of the ions appears to be independent of whether the reactant ions were generated by electron impact at 25 or 50 eV. The product distribution of each ion reaction was also studied as a function of the reactant translational energy. In summary, the data indicate that CF_3^+ will be the dominant ion in the ion flux reaching a substrate surface under many plasma conditions at the mtorr and higher pressures using C_3F_8 and C_3F_8/Ar mixtures.

REACTIONS OF O^+ WITH N_2 AND NO: RECOIL VELOCITY MEASUREMENTS IN A GUIDED-ION BEAM EXPERIMENT

D. Levandier and Y.-H. Chiu, Boston College, Newton, MA 02159, and S. Pullins and R. Dressler, Air Force Research Laboratory, Hanscom AFB, MA 01731 (Presented at the *52nd Annual Gaseous Electronics Conference*, Held in Norfolk VA, October 1999).

Previous studies of the reactions of O^+ with N_2 and NO indicate very small rates at thermal energies, with dramatic increases in reaction efficiency at higher collision energy. Recent interest in high pressure air plasmas and other extreme environments has led to the need for better characterization of these unusual exothermic reactions in the near-thermal to hyperthermal energy range, especially with regard to product state distributions. We have used the octopole guided-ion beam method to measure time-of-flight (TOF) spectra of the NO^+ produced in the reactions of ground state $O^+ + N_2$ and $O^+ + NO$. The velocity-transformed TOF data indicate more than one mechanism for both reactions. This presentation will discuss the more remarkable features of these results, including the complex-mediated $O^+ + N_2$ mechanism at hyperthermal collision energies. Where possible, the results are analyzed with the aid of the osculating complex model of chemical reaction and are compared to statistical theory.

CONCERNING THE CHEMICAL REACTIVITY OF THE ICE SURFACE

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Our research group has been examining chemical reactions on the surface of ice. The motivation has been to help develop a better understanding of the heterogeneous reactions that occur in the atmosphere and lead to the seasonal loss of ozone over the poles. In the laboratory we simulate the surface of these atmospheric ice particles, known as Polar Stratospheric Clouds or PSCs, using thin films of pure water ice. The interactions of reactive species with the ice surface is monitored using infrared transmission spectroscopy. During this talk we will present our most recent results concerning the chemical reactivity of the ice surface with HCl, HNO_3 and the acid-base reaction $HCl + NH_3$. From these studies we have discovered that the chemical reactivity of the ice changes as the mobility (or availability) of water at the surface changes.

RECOMBINATION COEFFICIENT MEASUREMENTS OF O AND N RADICALS

H. Singh, J. Coburn and D. Graves, University of California, Berkeley CA (Presented at the *52nd Annual Gaseous Electronics Conference*, Held in Norfolk VA, October 1999).

Surface recombination of radicals in low pressure high-density plasmas has direct influence on the neutral and ionic composition of the plasma. While electron impact dissociation of molecules is the dominant mechanism for creation of radicals, the surface recombination of radicals is often expected to be the dominant loss mechanism. We have a combination of measurements and a model to determine the recombination coefficients of O and N, to O_2 and N_2, respectively, on the stainless steel walls of our inductively coupled plasma chamber. The radial variation of the electron energy distribution function (EEDF) is measured using a tuned, cylindrical Langmuir probe. The number density of the molecular species is measured using line-of-sight modulated beam mass spectrometry. The mass spectrometer is differentially pumped in three stages to ensure a good beam to background signal ratio. The radical absolute number density is measured using appearance potential mass spectrometry with the aforementioned mass spectrometer. The recombination coefficient is calculated using a balance of the volume-generation and surface-loss rates of the radicals in the plasma. The generation rate of the radicals is calculated using the number density measurements of the parent molecule and the spatially resolved EEDFs. At approximately 330 K on stainless steel, the recombination coefficient for O is 0.16, and recombination coefficient for N is 0.07.

PARTICLE NUCLEATION IN ACETYLENE RADIOFREQUENCY PLASMAS

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(Presented at the *52nd Annual Gaseous Electronics Conference*, Held in Norfolk VA, October 1999).

The formation, growth and transport of sub-micron particles are critical issues in many plasma processes. The theory of gas phase nucleation of particles in plasmas is still in an early stage. It is commonly assumed that clustering in plasmas occurs through addition of growth species and formation of linear molecules. However, we believe that the formation of cyclic structures is an underlying theme of particle generation in plasmas. A chemical model describing the clustering kinetics in a low pressure acetylene radiofrequency discharge has been developed. The gas phase chemistry includes neutral-neutral reactions and electron-induced H-abstraction. In addition, diffusion losses to the reactor walls are considered. The model predicts the time evolution of species concentrations and chemical reaction rates, and gives the preferred clustering pathways. Even at room temperature the amount of produced polycyclic aromatic hydrocarbons (PAH) in the gas phase is considerable and strongly temperature dependent. Keeping the acetylene concentration constant, a balance between the species production by acetylene decomposition and diffusion losses is reached. The current chemical model will be extended by including negative ions, which have a long residence time in the plasma.

SPECTROSCOPY OF Na AND NOBLE GAS MIXTURES: PRECISE MEASUREMENTS OF ABSORPTION CROSS SECTION

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The absorption and emission of light by gases at high pressures are significantly influenced by atomic collisions, which result not only in atomic line broadening but also lead to very broad, essentially molecular spectra with rich rotational-vibrational structure and satellite features due to formation of molecules and quasi-molecules. We report new experimental results on the spectroscopy of sodium vapor and noble gas mixtures, which are compared with recent theoretical calculations. In order to perform the most stringent tests of the theoretical calculations, absolute values of absorption cross section are measured in the range 410 to 780 nm with better than 0.01 nm resolution. A special absorption cell was designed for this purpose. To determine accurately the sodium concentration in the mixture, the cell is placed in the test arm of a Mach-Zender interferometer and the 'hook' method in the vicinity of the Na line is applied. The concentration of noble gas is determined from pressure and temperature measurements.

SEMIEMPIRICAL SELF-CONSISTENT FIELD CONFIGURATION INTERACTION CALCULATIONS OF THE ELECTRONIC SPECTROSCOPY OF THE V_2, VNb, AND Nb_2 DIMER MOLECULES

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The ground and excited electronic states of the dimers V_2, VNb, and Nb_2 have been studied using the Intermediate Neglect of Differential Overlap Model for molecular optical properties (INDO/S). States are assigned on the basis of calculated transition energies, oscillator strengths and spin-orbit splittings. All three dimers are found to have $^3\sigma_g^-$ ground states arising from half-filled $d\delta_g$ shells, in accord with previous experimental and theoretical predictions. The large second-order spin-orbit splitting of this state is accurately predicted by our calculations. For V_2 two observed $^3\sigma_u^- \leftarrow {}^3\sigma_g^-$ transitions that have been observed in molecular beam spectroscopy are assigned as primarily $\sigma_u \leftarrow \sigma_g$ in character, and the observed $^3\pi_u \leftarrow {}^3\sigma_g^-$ transition is assigned as $d\pi_u \leftarrow d\delta_g$. Tentative assignments of a band system observed for VNb and a number of band systems observed for Nb_2 are also made.

QUANTUM MECHANICAL AND QUASICLASSICAL TRAJECTORY SURFACE HOPPING STUDIES OF THE ELECTRONICALLY NONADIABATIC PREDISSOCIATION OF THE A-STATE OF NaH_2

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Fully coupled quantum mechanical scattering calculations and adiabatic uncoupled bound-state calculations are used to identify Feshbach funnel resonances that correspond to long-lived exciplexes in the A-state of NaH_2, and the scattering calculations are used to determine their partial and total widths. The total widths determine the lifetimes, and the partial widths determine the branching probabilities for competing decay mechanisms. We compare the quantum mechanical calculations of the resonance lifetimes and the average final vibrational and rotational quantum numbers of the decay product, $H_2(v',j')$, to trajectory surface hopping calculations carried out by various prescriptions for the hopping event. Tully's fewest switches algorithm is used for the trajectory surface hopping calculations, and we present a new strategy for adaptive stepsize control that dramatically improves the convergence of the numerical propagation of the solution of the coupled classical and quantum mechanical differential equations. We performed the trajectory surface hopping calculations with four prescriptions for the hopping vector that is used for adjusting the momentum at hopping events. These include changing the momentum along the nonadiabatic coupling vector (d), along the gradient of the difference in the adiabatic energies of the two states (g), and along two new vectors that we describe as the rotated-d and rotated-g vectors. We show that the dynamics obtained from the d and g prescriptions are significantly different from each other, and we show that the d prescription agrees better with the quantum results. The results of the rotated methods show systematic deviations from the non-rotated results, and in general the error of the non-rotated methods is smaller. The non-rotated TFS-d method is thus the most accurate method for this system, which was selected for detailed study precisely because of the fact that it is more sensitive to the choice of hopping vector than previously studied systems.

SPATIAL DISTRIBUTION MEASUREMENTS OF ABSOLUTE CF_n (n=1-2) RADICAL DENSITIES USING SINGLE PATH INFRARED DIODE LASER ABSORPTION SPECTROSCOPY AND LASER INDUCED FLUORESCENCE TECHNIQUE

M. Ito, M. Nakamura, M. Hori and T. Goto, Nagoya University, and N. Ishii, Tokyo Electron Ltd. (Presented at the *52nd Annual Gaseous Electronics Conference*, Held in Norfolk VA, October 1999).

We have developed a novel measurement method for obtaining spatial distributions of absolute radial densities in plasma reactors. This measurement method consists of a laser induced fluorescence (LIF) technique and a single path infrared laser absorption spectroscopy (SP-IRLAS). The measurements using the SP-IRLAS and the LIF can be carried out at the same time only by changing the laser beams. The

laser beam for the SP-IRLAS goes through the same path as the beam for the LIF does in the plasma reactor. Therefore, the absolute densities obtained by the SP-IRLAS are the values averaged on the exact same optical path as the LIF laser beam goes through. By using these values, the relative spatial distributions obtained by the LIF are easily converted to the absolute ones with high reliability. This method has been successfully applied to the spatial distribution measurement of absolute CF and CF_2 radicals in electron cyclotron resonance C_4F_8 plasmas. From the results obtained, it was found that CF radical densities were higher than CF_2 ones in the plasma region while lower out of the region.

ON THE HYDROCARBON CHEMISTRY IN H_2/Ar/O_2 MICROWAVE PLASMAS

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Low pressure, non-equilibrium, molecular plasmas are of great interest in the field of plasma processing and technology because of their high chemical reactivity. To extend the understanding of the main chemical processes in H_2/Ar/O_2 plasmas containing small amounts of methane or methanol, tunable infrared diode laser absorption spectroscopy has been used. The experimental arrangement consists of a diode laser spectrometer and a planar microwave discharge reactor (1.5 kW and 1.5 mbar). The ground state concentrations of various species have been measured for different H_2/O_2 ratios. These include the methyl radical, related hydrocarbons and small molecules containing oxygen. The degree of dissociation of methane or methanol was between 62 and 93%. Absolute concentrations of the methyl radical were between 10^{10} and 10^{11} cm^{-3}. For plasmas studied in the absence of oxygen the experimental results were compared with results obtained by model calculations of the plasma chemistry. The model takes into account 12 molecular species and 57 reactions, where improved rate coefficients for the relevant electron collision processes were used. Good agreement is found between measured and calculated concentrations.

DEVELOPMENT OF VACUUM ULTRAVIOLET ABSORPTION SPECTROSCOPY USING HIGH PRESSURE H_2 MICRODISCHARGE HOLLOW CATHODE LAMP FOR MEASUREMENTS OF H ATOM DENSITY IN PLASMAS

S. Takashima, M. Hori, A. Kono and T. Goto, Nagoya University, M. Ito, Wakayama University, and K. Yoneda, Nippon Laser & Electronics Laboratory (Presented at the *52nd Annual Gaseous Electronics Conference*, Held in Norfolk VA, October 1999).

H atoms play an important role in process plasmas. We have newly developed a high pressure H_2 microdischarge hollow cathode lamp (MHCL) as a light source for vacuum ultraviolet absorption spectroscopy (VUVAS). The transition line used for the measurement was Lyman-α. For MHCL, He gas containing a small amount of H_2 gas were employed. The total gas pressure was about 88 kPa. MHCL generates a point-source-like emission from the hollow 0.1 mm in diameter. MHCL was designed to prevent the emission profile broadening due to fast H atoms arising from the dissociation of H_2. Moreover, the self-absorption of MHCL was successfully reduced by decreasing the H_2 partial pressure below 7.0 Pa. From the measured results of the absorption intensity at Lyman-α as a function of the radiofrequency power in inductively coupled H_2 plasmas (H_2-ICPs), the spectral profile of MHCL was estimated to be the Voigt profile with the Doppler width corresponding to an H atom temperature of 300 K and the Lorentz width two times as large as the Doppler width. Using VUVAS employing MHCL, absolute densities of H atoms in H_2-ICPs were measured. The absolute density of H atoms was 6×10^{11} cm^{-3} at a pressure of 1.33 Pa and a radiofrequency power level of 100 W.

LASER ABSORPTION MEASUREMENT OF ATOMIC OXYGEN CONCENTRATIONS IN A dc CORONA DISCHARGE

M.-A. Bratescu, M. Ohkubo, T. Kamada and Y. Sakai, Hokkaido University, Japan (Presented at the *52nd Annual Gaseous Electronics Conference*, Held in Norfolk VA, October 1999).

The atomic oxygen concentrations in both positive and negative corona discharges were measured as functions of the discharge current I, gas pressure p, electrode distance d and fraction k of oxygen in gas mixtures. Two methods of laser absorption spectroscopy, classical absorption (LA) and plasma modulation (PM) techniques, were used to study the spatial distribution of $O(^5S_2^0)$ excited state density in the discharge in gas mixtures (He/O_2 and air). LA method was used to calibrate the PM signal. The high sensitivity of PM method allows measuring oxygen density of about 10^6 cm^{-3}. Atomic oxygen transition from $O(^5S_2^0)$ to $O(^5P_{1,2,3})$ at 777.408, 777.631 and 777.753 nm can be obtained with commercially available infrared laser diodes. The atomic oxygen density in the vicinity of the tip electrode decreases with increasing p (gas pressure) for d=1 cm. The density is $3x10^7$ cm^{-3} at 25 torr.cm and $3.5x10^6$ cm^{-3} at 75 torr.cm for I=3 mA and p=50 torr. For k<0.01% in He/O_2 the atomic oxygen density between 10^9 cm^{-3} and 10^{10} cm^{-3} was shown to be given by high O_2 dissociation.

Cavity Ringdown Spectroscopy of Etching Plasmas

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Many of the reactive species of interest in etching plasmas absorb light in the ultraviolet spectral region (200-300 nm). Measurement of these weak absorbances (10^{-2}-10^{-4} for a single pass) allows their absolute concentration to be determined. Previously, low-resolution spectra have been obtained using broad-band absorption spectroscopy, using a Xe arc lamp as the light source and a small monochromator equipped with a CCD Camera. Here we report high-resolution measurements using the recently developed Cavity Ringdown Spectroscopy (CRDS) technique. The pulsed tunable output of an excimer pumped double dye laser was injected into a high-Q optical cavity in which the plasma is included. The absorbance as a function of wavelength is then deduced from the lifetime of the light pulse in the cavity. This technique offers the possibility of real-time (1 s) absolute concentration measurements. Results have been obtained for the detection of CF, CF_2, AlF and SiF_2 radicals in capacitively-coupled radiofrequency plasmas in fluorocarbon gases. However, the deduction of absolute concentrations from CRDS spectra is complicated by the phenomenon of non-single exponential decays when the linewidth of the laser is greater than that of the transition observed.

Detection of CH in an Expanding Ar/Acetylene Plasma Using Cavity Ringdown Absorption Spectroscopy

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Cavity Ringdown absorption spectroscopy is used to measure the methylidyne (CH) radical in an Ar/acetylene plasma. The acetylene is injected in an Ar plasma that expands from a cascaded arc, working at sub-atmospheric pressure, into a low pressure vessel. The rotational spectrum of the $A^2\Delta(v'=0)\leftarrow X^2\Pi(v''=0)$ transition around 430 nm is recorded to determine the total CH ground state density, both as function of the current through the arc and as function of the injected acetylene flow. Total ground state densities between $0.5.10^{17}$ and 6.10^{18} m^{-3} are detected. A simple plug-down model can qualitatively describe the measured trends in the CH density in both current and flow.

Determination of Species Concentrations and Temperatures in Chlorine Inductively Coupled Plasmas

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Concentrations of neutral (Cl and Cl_2) and charged (n_e, $n_{Cl}{}^+$, $n_{Cl2}{}^+$) species are determined for a broad range of pressure and power conditions in an inductively-coupled plasma reactor by a combination of optical emission spectroscopy, Langmuir probe and laser induced fluorescence. In the plasmas operated in a capacitively-coupled mode (at low source power) the dominant ion is $Cl_2{}^+$. When power is increased and the plasma is operated in an inductively-coupled mode, the dominant ion is Cl^+. This is mainly a consequence of a low degree of dissociation of molecular chlorine at lower power and higher degree of dissociation at high power. We also carried out zero-dimensional modeling for both neutral and charged species that reproduced their dependence on pressure and power. The density of negative ions is determined both from experiment (through the difference of positive ion and electron densities) and modeling. Electron temperature (T_e) is determined by Langmuir probe and trace-rare gases optical emission spectroscopy. Differences in values of T_e between the two techniques are explained through derivations of the electron energy distribution function from Maxwellian behavior.

In situ Diagnostics of Highly Excited Hydrogen Molecules by LIF in the Vacuum Ultraviolet

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(Presented at the *52nd Annual Gaseous Electronics Conference*, Held in Norfolk VA, October 1999).

The population dynamics of low temperature hydrogen plasmas, though extensively treated in simulations, is still lacking complete experimental verification. This applies especially to the role of highly excited molecules in the electronic ground state, since the population of states with $v''>8$, considered of decisive importance for the generation of negative ions by the process of dissociative attachment, has been inaccessible for in situ diagnostics so far. Spatially resolved quantitative determination of their population in the plasma of a magnetic multipole source has now become possible by Laser Induced Fluorescence spectroscopy (LIF) in the vacuum ultraviolet. Populations with rotational resolution are obtained up to $v''=13$ with good signal-to-noise ratio. It is furthermore possible to follow the decay of the populations as a function of time after fast current shut-off. 1/e times ranging from milliseconds at small v'' down to several 10 microseconds at the highest states are found.

Optical Measurements of Atomic and Molecular Species in a Pulsed Radiofrequency Discharge in Nitrogen

S.F. Adams and C.A. DeJoseph Jr, Air Force Research Laboratory, Wright-Patterson AFB, OH, and T.A. Miller, The Ohio State University, Columbus, OH (Presented at the *52nd Annual Gaseous Electronics Conference*, Held in Norfolk VA, October 1999).

Emission spectroscopy and LIF have been used to study the heavy particle kinetics in a pulsed, parallel-plate radiofrequency discharge in nitrogen. A two-photon LIF technique utilizing 207 nm radiation was used to detect ground state N-atoms, while single-photon LIF was applied to the detection of $N_2(A^3\Sigma_u^+)$ and $N_2(B^3\Pi_g)$ excited molecular states. Emission spectroscopy was used to gain additional information on the molecular states. These optical techniques were used to monitor temporal and spatial changes in the species concentrations. The absolute N atom concentration, determined by titration, allowed an absolute density calibration of each of the molecular species by coupling the temporal LIF and emission measurements with known rate constants of several heavy particle reactions occurring in the post discharge. The measurements, coupled with a simple numerical model, allowed absolute densities of some species, such as $N_2(X^1\Sigma_g^+, v \geq 5)$, to be determined in spite of an inability to detect the species by optical diagnostics. Results will be shown for a variety of pulsed radiofrequency discharge conditions.

LIF OF OH RADICALS IN A DIELECTRIC-BARRIER DISCHARGE

R. Sankaranarayanan, B. Pashaie and S. Dhali, Southern Illinois University, Carbondale, IL 62901 (Presented at the *52nd Annual Gaseous Electronics Conference*, Held in Norfolk VA, October 1999).

We present the results of laser induced fluorescence (LIF) measurements of OH radicals in a dielectric-barrier discharge. The discharge consists of a simple dielectric-barrier with one glass dielectric excited with a frequency in the range of 1-3 kHz. A YAG-pumped tunable dye laser is doubled to produce the excitation at 282 nm. The laser beam excites the OH molecule from the v″=0 of the ground electronic state to v′=1 of the excited electronic state. The broadband radiation due to the (1,1) transition is recorded in the 312-330 nm range. A gated CCD camera is used to record the LIF with spatial resolution. Results of OH concentration with variation in power supply voltage, oxygen concentration, and flow will be presented. Results show that with increase in power supply voltage, there is a drop in OH concentration. This is likely due to the change in the nature of the discharge at higher powers.

RAMAN MEASUREMENTS OF N_2, CO AND O_2 VIBRATIONAL STATE DISTRIBUTIONS IN LASER SUSTAINED, HIGH PRESSURE NON-EQUILIBRIUM DISCHARGES

W. Lee, I.V. Adamovich and W. Lempert, The Ohio State University, Columbus, OH 43210 (Presented at the *52nd Annual Gaseous Electronics Conference*, Held in Norfolk VA, October 1999).

It is well known that the CO laser can be used to initiate and sustain electron production in pure CO at low to modest translational temperature. However, in the presence of common diatomic buffer gases such as O_2 and N_2, interspecies vibrational (V-V) energy transfer is known to ‘quench' the highly excited CO vibrational distribution which is critical for the production of free electrons. Theoretically, V-V exchange rates between CO and typical buffer gases are not well quantified and hence, electron production cannot be accurately predicted. In this paper, we will present new experimental results which quantify the vibrational state distribution functions of the key diatomic plasma species N_2, O_2 and CO in high pressure, laser-sustained nonequilibrium discharges. For the homonuclear diatomics, N_2 and O_2, the measurements will be performed using spontaneous Raman scattering. For CO, measurements will be performed both with Raman scattering and spontaneous FTIR emission spectroscopy. The focus of the paper will be two-fold: First, diagnostic issues pertinent to application of Raman spectroscopy to high pressure discharges will be described in some detail. Second, experimental data will be compared to predictions from detailed kinetic ‘Master Equation' modeling, emphasizing the influence of CO-O_2 and N_2-O_2 vibrational energy transfer on CO vibrational excitation and, ultimately, free electron production. Measurements will be presented in N_2/CO plasmas, N_2/CO/O_2 plasmas and Ar/CO/O_2 plasmas.

3-D TIME-RESOLVED FTIR SPECTROSCOPY STUDIES OF PHOTOCHEMISTRY AT 193.3 nm

J.D. Wrobel, M. Green and W.M. Jackson, Chemistry Department, University of California, Davis, 1-Shields Avenue, Davis, CA 95616, Fax (530) 752-8995, wrobel@chem.ucdavis.edu, and I.A. McLaren, McLaren Research, 190 Gladys Avenue, Suite A, Mountain View, CA 94043 (Presented at the *218th National Meeting of the American Chemical Society*, Held in New Orleans LA, August 1999).

Step-scan time-resolved FTIR emission spectroscopy was used to obtain infrared spectra from vibrationally excited CH_3, C_2H_6, CO, C_2H and C_2 produced during the photolysis of acetone and acetylene at 193.3 nm. The spectra were collected in the region between 4500 and 2000 cm^{-1} with spectral and time resolutions as high as 1 cm^{-1} and 1 μs, respectively. The time and pressure dependences of the ethane emission indicate that it arises from the recombination of methyl radicals. The (0-0) band of the ($B^1\delta \rightarrow A^1\pi$) is observed when the laser is focused in acetylene. The intensity of this C_2 spectrum confirm that nonadiabatic processes are important in the photochemistry of acetylene.

IMAGING RADICAL DISSOCIATION DYNAMICS

M. Ahmed, D.S. Peterka and A.G. Suits, Chemical Sciences Division, Ernest Orlando Lawrence Berkeley National Laboratory, Berkeley, CA 94720, Fax (510) 486-5664, musa@leea.lbl.gov (Presented at the *218th National Meeting of the American Chemical Society*, Held in New Orleans LA, August 1999).

The study of the dynamics of photodissociation can give detailed information on the nature of potential energy surfaces and the coupling between them, the structure of the transition state, and the identity, branching fractions and thermodynamics of the dissociation pathways. We have studied photodissociation of a number of hydrocarbon free radicals generated under well defined conditions in a supersonic molecular beam using velocity map imaging. The radicals were generated via laser-photolysis using 193 nm light in the collision region of a pulsed nozzle expansion. Photodissociation of the radical and subsequent resonant ionization of the H atom photofragment were carried out using 243 nm light. In the photodissociation of the vinyl radical (C_2H_3), the primary product is singlet vinylidene. In addition, a minor contribution is seen which is assigned to triplet acetylene. The heat of formation of vinylidene obtained from the experiment is in agreement with literature values, and we also report the first experimental excitation energy for the lowest triplet state of acetylene. We have also studied the dissociation dynamics of a number of other hydrocarbon radicals; the results will be presented at this symposium.

FEMTOSECOND STUDIES OF DISSOCIATION DYNAMICS USING 3-D IMAGING TECHNIQUES

J.A. Davies, Department of Chemistry and Biochemistry, University of California, San Diego, 9500 Gilman Drive, La Jolla, CA 92093, Fax (925) 294-2276, jadavie@sandia.gov, and Carl C. Hayden, Combustion Research Facility, Sandia National Laboratories, P.O. Box 969, Livermore, CA 94551 (Presented at the *218th National Meeting of the American Chemical Society*, Held in New Orleans LA, August 1999).

Dissociation dynamics are studied using a new femtosecond time-resolved photoionization probe technique that combines photoelectron-photoion coincidence detection with three-dimensional energy- and angle-resolved imaging. Initial studies have focused on the dissociation process that occurs during dissociative multiphoton ionization (DMI) of NO_2 induced by femtosecond laser pulses centered at 375.3 nm. The dominant DMI pathway is identified as three-photon excitation to a repulsive potential surface correlating to $NO(C^2\Pi)+O(^3P)$ followed by one-photon ionization to $NO^+(X^1\Sigma^+)$. Dissociation along this surface is followed on a femtosecond timescale. Three-dimensional angular correlations between the photoions and photoelectrons have been measured and will be presented at the meeting.

NONADIABATIC DISSOCIATION DYNAMICS OF CH_2BrCl

S.W. North, W.S. McGivern, R. Li and P. Zou, Department of Chemistry, Texas A&M University, P.O. Box 300012, College Station, TX 77842, Fax (409) 845-2971, north@mail.chem.tamu.edu (Presented at the *218th National Meeting of the American Chemical Society*, Held in New Orleans LA, August 1999).

The photodissociation dynamics of CH_2BrCl have been studied using resonance-enhanced multiphoton ionization time-of-flight mass spectrometry. Polarization dependent time-of-flight profiles were collected for a range of wavelengths from 248-268 nm, corresponding to the red wing of the absorption spectrum. Forward convolution fits to the data have provided translational energy distributions and anisotropy parameters over the entire wavelength range for both $Br(^2P_{3/2})$ and $Br^*(^2P_{1/2})$. The average translational energies for the Br and Br* channels are 20 and 23 kcal/mol respectively. The measured anisotropy parameters indicate that both channels arise preferentially from a parallel transition and that the contribution of this transition increases with wavelength. Nonadiabatic transitions play a smaller role in CH_2BrCl dissociation than in its monohalogenated analogs. We propose that this difference is the result of the lower symmetry, lower radial velocity, and greater reduced mass of CH_2BrCl, and it is discussed in terms of a one-dimensional Landau-Zener model. A C-Br bond dissociation energy of 72.0 kcal/mol in CH_2BrCl was also calculated using ab initio methods at the MP2/cc-pVtz//MP2/cc-pVdz level.

PHOTODISSOCIATION DYNAMICS OF THE CNN FREE RADICAL

R.T. Bise, A. Hoops, H.S. Choi and D.M. Neumark, Department of Chemistry, University of California, Berkeley, CA 94720, Fax (510) 642-6262, ryan@radon.cchem.berkeley.edu (Presented at the *218th National Meeting of the American Chemical Society*, Held in New Orleans LA, August 1999).

The spectroscopy and photodissociation dynamics of the $A(^3\pi)$ and $B(^3\sigma)$ states of the CNN radical have been investigated by fast beam photofragment translational spectroscopy. Vibronic transitions located more than 1000 cm^{-1} above the (A-X) origin were found to predissociate. Photofragment yield spectra for the (B-X) band between 40800 and 45460 cm^{-1} display resolved vibrational progressions with peak spacing of 1000 cm^{-1} corresponding to symmetric stretch progressions. The ground state products $C(^3P)+N_2$ were found to be the major photodissociation channel for both the A and B-states. The translational energy distributions for the $A(^3\pi)$ state are bimodal with high and low translational energy components. The distributions for the $B(^3\sigma)$ state reveal partially resolved vibrational structure for the N_2 photofragment and indicate extensive vibrational and rotational excitation of this fragment. The results provide a more accurate heat of formation for CNN (6.210($\pm$0.030 eV)) and suggest that bent geometries are involved in the dissociation mechanism.

SPECIFICITY AND NONSPECIFICITY IN THE CO_2-LASER SENSITIZED REACTION OF TETRACHLOROETHENE
B.L. Earl and R.L. Titus, Department of Chemistry, University of Nevada at Las Vegas, Las Vegas, NV 89154, Fax (702) 895-4072, bearl@nevadaledu (Presented at the *218th National Meeting of the American Chemical Society*, Held in New Orleans LA, August 1999).

Previous workers have investigated the reaction of tetrachloroethene using thermal initiation and CO_2 laser initiation via sensitizing species which absorb the laser radiation. In both instances, the principal product was found to be hexachlorobenzene. One group reported evidence of laser specificity in this reaction, in that BCl_3 acted as a sensitizer to produce hexachlorobenzene as the main product, but SF_6 and BBr_3 did not. We have found that specificity is highly dependent on reaction conditions. We reproduced the previous results using similar experimental conditions, but under different conditions we found that the specificity disappeared, with all three sensitizers which we used (BCl_3, SF_6, and SiF_4) sensitizing the reaction to produce mainly hexachlorobenzene. There were some differences among the sensitizers as, for example, the fact that SF_6 produced the most nearly pure hexachlorobenzene product.

ELECTRONICALLY NONADIABATIC TRANSITIONS IN MOLECULAR PHOTODISSOCIATION PROCESSES
G.G. Balint-Kurti, United Kingdom, Gabriel.Balint-Kurti@Bristol.ac.uk (Presented at the *218th National Meeting of the American Chemical Society*, Held in New Orleans LA, August 1999).

The theory of photodissociation processes using quantum wavepacket dynamics will be reviewed. Applications of the theory will be presented for two different systems. For H_2O the second absorption band (B^1A_1-$^1A_1$) will be discussed where the electronically nonadiabatic transition occurs via a conical intersection in linear geometry. Detailed results will also be presented for the photodissociation of HI, where spin-orbit coupling leads to the production of two different electronic states of iodine, each with its own angular distribution. For HOCl new theory will be presented for the correlated scattering angle dependent polarized distributions of the OH λ-doublet states and the spin-orbit states of the Cl atoms.

EMPIRICAL VALENCE BOND APPROACH FOR ACETYL RADICAL DISSOCIATION DYNAMICS
M. Ito and M. Aoyagi, Computer Center, Institute for Molecular Science, 38 Saigohnaka, Myodaiji, Okazaki, 444-0867, Japan, Fax (81)-564-55-7025, mito@ims.ac.jp (Presented at the *218th National Meeting of the American Chemical Society*, Held in New Orleans LA, August 1999).

It was shown that the RRKM dissociation rate constant k(E) of acetyl radicals did not represent the experimental values. We employed the empirical valence bond methodology to model this reaction which permits the construction of the potential energy surface in an accurate and numerically efficient way. Our model Hamiltonian is separated into the reactive part H_spin and the non-reactive part V. H_spin consists of spin operators localized to the reactive bonds, while V is just a diagonal matrix whose element is expressed as the sum of intramolecular contributions in each electronic structure. The parameters were fit to the UHF/MP2 calculations in various conformations around the dissociation reaction path and the resulting energies show good agreement with ab initio values. Our model was furthermore applied in a molecular dynamics simulation where the forces acting on the atoms were derived by diagonalizing the electronic Hamiltonian.

Photofragment Imaging Studies of Unimolecular Decomposition

A. Sanov, Department of Chemistry, University of Arizona, Tucson, AZ 85721, Fax (303) 492-5235, sanov@jilau1.colorado.edu, and M. Zyrianov, T. Droz-Georget and H. Reisler, Department of Chemistry, University of Southern California, Los Angeles, CA 90089 (Presented at the *218th National Meeting of the American Chemical Society*, Held in New Orleans LA, August 1999).

The unimolecular decomposition of jet-cooled HNCO via three competing channels has been investigated following photoexcitation to the S_1 state in energy regions where one to three channels are open. The role of photofragment ion imaging in determining reaction barriers, elucidating the mechanisms of surface crossings, and identifying different reactive pathways characterized by different time scales will be emphasized. It is demonstrated that in mechanistic studies, experiments near thresholds of specific channels are particularly revealing. The results are discussed in terms of vibronic levels of mixed electronic character coupled directly or via radiationless decay to the various continua and exhibiting several distinct time scales. The determination of scalar and vector photofragment properties are crucial to the understanding of the photophysics and photochemistry. Time permitting, the effect of fragment rotational excitation on angular distributions will be discussed, as well as novel applications of photoelectron imaging to time-resolved studies of electronic structure evolution in chemical reactions involving negative ions and clusters.

Quantum Chemical Studies of the Dissociation Pathways of Alkoxy Radicals Formed in the Atmospheric Degradation of Isoprene

T.S. Dibble, Chemistry Department, State University of New York, Environmental Science and Forestry, 1 Forestry Drive, Syracuse, NY 13210, Fax (315) 470-6856, tsdibble@mailbox.syr.edu (Presented at the *218th National Meeting of the American Chemical Society*, Held in New Orleans LA, August 1999).

Isoprene is one of the most important non-methane organic compounds in tropospheric chemistry, yet its degradation pathways are poorly understood. The fates of alkoxy radicals formed in isoprene oxidation are a large part of this mystery. Alkoxy radicals formed in the first stages of the OH-initiated degradation of isoprene are studied at the B3LYP/6-311G(2df) level of theory; some processes also are examined at the CBS-4 level of theory. For the four β-hydroxyalkoxy radicals that are expected to be formed, C-C bond fission has a very low barrier (1-2 kcal/mole) and is likely to dominate the chemistry. These radicals probably also possess internal hydrogen bonds which play a role in the transition state. Two δ-hydroxyalkoxy radicals will also be formed, but for these species C-C bond fission may be too endothermic (15-20 kcal/mole) for this pathway to be important. Isomerization and C-H bond fission pathways will also be discussed.

Energetic and Structural Features of the CH_4+O(^{3}P)®CH_3+OH Abstraction Reaction: Does Perturbation Theory from a Multiconfiguration Reference State (Finally) Provide a Balanced Treatment of Transition States?

O. Roberto-Neto, Instituto de Estudos Avancados, Centro Tecnico Aerospacial, Sao Jose dos Campos, Sao Paulo, 12228-840 Brazil, F.B.C. Machado, Departamento de Quica, Instituto Technologico de Aeronautica, Centro Tecnico Aerospacial, Sao Jose dos Campos, Sao Paulo, 12228-840 Brazil, and D.G. Truhlar, Department of Chemistry and Supercomputer Institute, University of Minnesota, Minneapolis, MN 55455 (to Appear in the *Journal of Chemical Physics*).

The stationary points of the $CH_4+O(^3P)\rightarrow CH_3+OH$ abstraction reaction have been identified at the fully optimized reaction space (FORS) level. For three sets of geometries (FORS plus unrestricted and restricted-open-shell Moller-Plesset second order perturbation theory), single-point calculations by unrestricted Moller-Plesset fourth order perturbation theory (UMP4), by unrestricted coupled cluster theory with single and double excitations and a quasiperturbative treatment of fourth- and fifth-order triple-excitation terms (CCDS(T)), and by multi-reference Moller-Plesset second order perturbation theory (MRMP2) were also performed for the classical barrier height and energy of the reaction.

Calculations carried out at the MRMP2/cc-pVTZ//FORS/cc-pVTZ level predict values for the forward vibrationally adiabatic barrier height and for the energy of the reaction at 0 K equal to 10.3 and 2.0 kcal/mol, respectively. This is in excellent agreement with experiments that show values of the activation energies in the range of 9 to 12 kcal/mol (at temperatures below 1500 K) and an energy of reaction equal to 1.8 kcal/mol. Expectation values of S^2, where S is total electron spin, and also the values the coefficients of the configuration state functions show that the reactants and the products of this reaction are well described by single-configuration reference states but that the transition structure has a much higher multi-configurational character. We conclude that MRMP2 may provide some light at the end of the tunnel in the long-standing quest for a method that includes nondynamical and dynamical correlation in a balanced way in the electronic wave function of open-shell transition states.

Quantum Chemical Studies of the Thermal Decomposition of Furan

K. Sendt, G.B. Bacskay and J.C. Mackie, Division of Physical and Theoretical Chemistry, School of Chemistry, University of Sydney, NSW, 2006, Australia, sendt_k@chem.usyd.edu.au (Presented at the *218th National Meeting of the American Chemical Society*, Held in New Orleans LA, August 1999).

Ab initio quantum chemical calculations have been performed in order to study the pyrolysis of furan in the temperature range 1100-1700 K. The potential energy surfaces of furan and related compounds have been computed using G2MP2 and CASPT2 methods, enabling the determination of the major reaction paths in the thermal decomposition of furan and the kinetic parameters for these paths.

The major decomposition routes for furan were found to occur via hydrogen migrations followed by ring opening to produce the experimentally determined products, namely CO, C_3H_4, CH_2CO and C_2H_2. The reaction pathway involving 3,2 H-migration was predicted to have an activation energy of 294 kJ mol^{-1}, producing CO and C_3H_4. The reaction pathway involving 2,3 H-migration was predicted to have an activation energy of 346 kJ mol^{-1}, producing CH_2CO and C_2H_2. The reaction pathways involving 3,4 H-migration or direct CO bond cleavage of furan were found to have negligible contribution to the overall reaction flux. The calculated and experimental rate constants for the disappearance of furan at a range of temperatures have been determined.

Crossed-Beam Studies of CO Rotational Energy Transfer

G.C. McBane, S. Antonova, A. Lin and A.P. Tsakotellis, Department of Chemistry, The Ohio State University, 100 W. 18th Avenue, Columbus, OH 43210, Fax (614) 292-1685, mcbane.2@osu.edu, and K.T. Lorenz and D.W. Chandler, Combustion Research Facility, Sandia National Laboratories, P.O. Box 969, Livermore, CA 94551 (Presented at the *218th National Meeting of the American Chemical Society*, Held in New Orleans LA, August 1999).

Rotational excitation of CO in collisions with He and Ne has been studied in crossed molecular beams. State-to-state differential cross sections have been determined by velocity mapping with (2+1) REMPI ionization of the scattered CO. Numerical simulation of the image data, extraction of differential cross sections from the experimental images, and comparisons with predictions of several high quality potential surfaces will be presented.

TECHNICAL MEETINGS

(Current Additions to this List are Indicated by a Diamond Bullet Marking)

JANUARY 6-8, 2000

4th ISHMT/ASME HEAT AND MASS TRANSFER CONFERENCE
Pune Maharashtta, India.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7284, Fax (212) 705-7143, http://www.asme.org

JANUARY 9-13, 2000

SYMPOSIUM ON ENERGY ENGINEERING IN THE 21st CENTURY
Hong Kong, China.

Information: Ping Cheng, Department of Mechanical Engineering, Hong Kong, University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong, (852) 2358-7182, Fax (852) 2358-1543, e-mail: mepcheng@ust.hk, or P. Takahashi, Hawaii Natural Energy Institute, University of Hawaii, Honolulu, HI 96822, (808) 956-8346, Fax (808) 956-2336, e-mail: ptakaha@uhccmvs.uhcc.hawaii.edu

JANUARY 9-13, 2000

PITZER MEMORIAL SYMPOSIUM ON THEORETICAL CHEMISTRY
Berkeley CA.

Information: W.H. Miller, Department of Chemistry, University of California, Berkeley CA 94720, e-mail: pitzer2000@cchem.berkeley.edu

JANUARY 10-13, 2000

38th AIAA AEROSPACE SCIENCES MEETING AND EXHIBIT
Reno NV.

Meeting has Symposia on:

- Aeroacoustics
- Aerodynamic Measurement Technology
- Applied Aerodynamics
- Atmospheric Flight Mechanics
- Microgravity Science and Space Processing
- Plasmadynamics and Lasers
- Propellants and Combustion
- Aerospace Power Systems
- Air-Breathing Propulsion
- Fluid Dynamics
- Intelligent Systems
- Interactive Computer Graphics
- Thermophysics

Information: Meetings Department, American Institute of Aeronautics and Astronautics, 1801 Alexander Bell Drive, Suite 500, Reston, VA 20191, (703) 264-7500 or (800) 639-2422, e-mail: custserv@aiaa.org, http://www.aiaa.org

JANUARY 10-15, 2000

WINTER CONFERENCE ON PLASMA SPECTROCHEM
Fort Lauderdale FL.

Information: R. Barnes, ICP Info Newsletter, P.O. Box 666, Hadley, MA 01003, e-mail: winterconf@chem.umass.edu

JANUARY 22-28, 2000

PHOTONICS WEST
San Jose CA.

Information: Meetings Department, SPIE, P.O. Box 10, Bellingham, WA 98227, (360) 676-3290, Fax (360) 647-1445, e-mail: spie@spie.org, http://www.spie.org

FEBRUARY 11-14, 2000

7th LASER APPLICATIONS TO CHEMICAL ANALYSIS MEETING: TOPICAL MEETING OF THE OPTICAL SOCIETY OF AMERICA
Santa Fe NM.

Topics will Include:
- Application of New Laser Sources to Analytical Spectroscopy
- Diode Laser Applications in Combustion, Industrial and Atmospheric Measurements
- Laser Diagnostics for Combustion
- Laser Based Detection Coupled to Microanalytical Separations
- Microoptical Systems for Chemical Analysis
- Laser Based Detection for High Density Chemical Sensing Arrays
- Development and Applications of Single-Molecule Spectroscopy
- Fluorescence Based Methods for Detection of Individual Bimolecules (Including Imaging)

Information: J.B. Jeffries, Molecular Physics Laboratory, SRI International, 333 Ravenswood Ave., Menlo Park, CA 94025, (650) 859-6341, Fax (650) 859-6196, e-mail: Jeffries@crvax.SRI.com, http://www.osa.org/mtg_conf/2000/lacea/
Deadline: Abstracts Due by September 22, 1999.

MARCH 5-8, 2000

8th INTERNATIONAL CONFERENCE ON NUMERICAL COMBUSTION
Amelia Island FL.

Conference Topics Include:
- Turbulence
- Kinetics
- Detonation
- Flames
- Pollution
- Microgravity
- Ignition
- Applications of Parallel Processing
- Tera-scale Computation of Combustion Applications

- Material Synthesis
- Droplets and Sprays
- Heterogeneous Combustion
- Energetic Materials (Propellants and Explosives)
- Engine and Furnace Combustion
- Fires
- Adaptive Numerical Methods
- Software Engineering for Combustion Applications

Invited Speakers Include:

- Premixed Turbulent Combustion: DNS into Modeling, R. Stewart Cant, University of Cambridge, United Kingdom
- Numerical Modeling of Combustion Control in Ramjets, Sergei Frolov, Semenov Institue of Chemical Physics, Russia
- Aerothermochemistry of Flames, Peter Lindstedt, Imperial College, United Kingdom
- Experimental Measurements of Solid Propellant Flame Structure for Model Validation, Timothy Parr, U.S. Naval Air Warfare Center
- Some New Developments in Pre-Mixed Gaseous Combustion, Gregory I. Sivashinsky, Tel Aviv University, Israel
- The Impact of the Accelerated Strategic Computing Initiative on Numerical Combustion, Charles K. Westbrook Lawrence Livermore National Laboratory

Information: Society for Industrial and Applied Mathematics, 3600 University Science Center, Philadelphia, PA 19104, http://www.siam.org/meetings/

♦ MARCH 5-9, 2000

2000 SPRING NATIONAL MEETING OF THE AMERICAN INSTITUTE OF CHEMICAL ENGINEERS ON ADVANCED NEW TECHNOLOGIES IN INDUSTRY
Atlanta GA.

Topics will Include:

- 12th Ethylene Producers Conference
- 34th Loss Prevention Conference
- 4th International Conference on Microreaction Technology
- 3rd International Conference on Refining Processes

Information: W.S. Winston Ho, Meeting Program Chair, Department of Chemical and Materials Engineering, 177 Anderson Hall, Lexington, KY 40506, (606) 257-4815, Fax (606) 323-1929, e-mail: wsho@engr.uky.edu

MARCH 6-9, 2000

SAE INTERNATIONAL CONGRESS AND EXPOSITION
Detroit MI.

Information: Society of Automotive Engineers, Inc., 400 Commonwealth Drive, Warrendale, PA 15096, (724) 776-4841, Fax (724) 776-5760, e-mail: meetings@sae.org, http://www.sae.org

♦ MARCH 12-14, 2000

ASTM COMMITTEE E-13 ON MOLECULAR SPECTROSCOPY
New Orleans LA.

Information: G. Collins, ASTM, (610) 832-9715, Fax (610) 832-9635, e-mail: gcollins@astm.org, http://www.astm.org

MARCH 12-17, 2000

THE PITTSBURGH CONFERENCE, PITTCON 2000
New Orleans LA.

Information: The Pittsburgh Conference, 300 Penn Center Boulevard, Suite 332, Pittsburgh, PA 15235, (412) 825-3220, Fax (412) 825-3224, e-mail: pittconinfo@pittcon.org, http://www.pittcon.org/

MARCH 13-14, 2000

SPRING MEETING OF THE WESTERN STATES SECTION OF THE COMBUSTION INSTITUTE
Colorado School of Mines, Golden CO.

Information: W.J. Pitz, L-353, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, CA 94551, (925) 422-7730, Fax (925) 422-2644, e-mail: pitz@llnl.gov, http://www.wssci.org/

MARCH 20-24, 2000

MARCH MEETING OF THE AMERICAN PHYSICAL SOCIETY
Minneapolis MN.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

MARCH 26-30, 2000

SPRING NATIONAL MEETING OF THE AMERICAN INSTITUTE OF CHEMICAL ENGINEERS
Atlanta GA.

Information: Meetings Department, American Institute of Chemical Engineers, United Engineering Center, 345 East 47th Street, New York, NY 10017, (212) 2705-7338 or (800) 242-4363, http://www.aiche.org

MARCH 26-31, 2000

219th NATIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
San Francisco CA.

Division of Analytical Chemistry:

- New Frontiers in Analytical Chemistry
- Analytical Problems of the 21st Century
- Limitations of Present Analytical Tools

T.R. Williams, College of Wooster, Wooster, OH 44691, (330) 263-2115, e-mail: williams@acs.wooster.edu

Division of Fuel Science:

- Fuel Science in the Year 2000: Where Do We Stand, Where Do We Go From Here?
  G.P. Huffman, 533 S. Limestone Street, Suite 111, University of Kentucky, Lexington, KY 40506-0043, (606) 257-4027, Fax (606) 257-7215 e-mail: cffls@pop.uky.edu
- Advances in F-T Chemistry
  B.H. Davis, Center for Applied Energy Research, University of Kentucky, Lexington, KY 40511, (606) 257-0251, Fax (606) 257-0302, e-mail: davis@alpha.caer.uky.edu
- Molecular Modeling of Solid-Fuel Reactions
  L.R. Radovic, Fuel Science Program, Pennsylvania State University, 217 Academic Projects Building, University Park, PA 16802, (814) 863-0594, Fax (814) 865-3075, e-mail: lrr3@psu.edu
- Applications of X-ray and Gamma Ray Techniques in Fuel Science
  K.A. Carrado, CHM/200, 9700 S. Cass Avenue, Argonne National Laboratory, Argonne, IL 60439-4831, (630) 252-7968, Fax (630) 252-9288, e-mail: kcarrado@anl.gov
- Particulate Matter and Fossil Fuel Combustion
  T.J. Feeley III, Department of Energy, Federal Energy Technology Center, P.O. Box 10940, Pittsburgh, PA 15236, (412) 892-6134, Fax (412) 892-5914, e-mail: feeley@fetc.doe.gov
- Solid Fuel Chemistry
  F. Huggins, South Limestone Street, Suite 111, University of Kentucky, Lexington, KY 40506, (606) 257-4045, Fax (606) 257-7215, e-mail: fhuggins@engr.uky.edu

Division of Petroleum Chemistry:

- New Chemistry of Fuel Additives
  D. Daly, Fuel Products, Strategic Technology, Lubrizol Co., 29400 Lakeland Blvd., Wickliffe, OH 44092, (440) 943-1200 ext. 4261, Fax (440) 943-9022, e-mail: dtd@lubrizol.com
- CO_2 Conversion and Utilization in Refinery and Chemical Processing
  C. Song, Pennsylvania State University, 209 Academic Projects Building, University Park, PA 16802, (814) 863-4466, Fax (814) 865-3075, e-mail: csong@psu.edu; A.M. Gaffney, DuPont Central R&D, Experimental Station, P.O. Box 80262, Wilmington, DE 19880, (302) 695-1800, Fax (302) 695-8347, e-mail: anne.m.gaffney@usa.dupont.com

Division of Physical Chemistry:

- Physical Chemistry at High Pressure and Temperature
  A.P. Alivisatos, Department of Chemistry, University of California, Berkeley CA 94720, (510) 643-7371, Fax (510) 642-6911, e-mail: alivis@uclink4.berkeley.edu; R. Jeanloz, Department of Geology & Geophysics, University of California, Berkeley CA 94720, (510) 642-2639, Fax (510) 643-9980, e-mail: jeanloz@uclink.berkeley.edu
- Atmospheric Chemistry (Harold Johnston Festschrift)
  C.E. Miller, Department of Chemistry, Haverford College, Haverford, PA 19041, (610) 896-1388, Fax (610) 896-4904, e-mail: cmiller@haverford.edu
- Potential Energy Surfaces: From Polyatomics to Macromolecules
  L.X. Dang, EMSL, Pacific Northwest National Laboratory, P.O. Box 999, Richland, WA 99352, (509) 375-2034, Fax (509) 375-6631, lx_dang@pnl.gov

Information: From the Individual Chairpersons or from Meetings Department, American Chemical Society, 1155 - 16th Street, NW, Washington, DC 20036, (202) 872-4396, Fax (202) 872-6128, e-mail: natlmtgs@acs.org

Deadline: 4 Copies of 150-Word Abstract (Original on ACS Abstract Form to Symposium Organizer by November 1, 1999 (Analytical and Physical Chemistry), October 15, 1999 (Fuel and Petroleum Chemistry).

MARCH 26-31, 2000

CORROSION/2000

Orlando FL.

Information: NACE Headquarters, Meetings Department, P.O. Box 218340, Houston, TX 77218, (281) 228-6200, Fax (281) 228-6300, http://www.nace.org

APRIL 3-6, 2000

3rd INTERNATIONAL SYMPOSIUM ON TURBULENCE, HEAT AND MASS TRANSFER
Nagoya, Japan.

Information: T. Tsuji, Symposium Secretary, Department of Mechanical Engineering, Nagoya Institute of Technology, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan, (81) 52-735-5333, Fax (81) 52-735-5359, e-mail: tsuji@heat.mech.nitech.ac.jp, http://heat.mech.nitech.ac.jp/thmt3/

♦ APRIL 3-6, 2000

41st AIAA/ASME/ASCE/AHS/ASC STRUCTURES, STRUCTURAL DYNAMICS AND MATERIALS CONFERENCE
Atlanta GA.

Information: M. Kamat, School of Aerospace Engineering, Georgia Institute of Technology, Atlanta, GA 30332, (404) 894-7439, Fax (404) 894-9313, e-mail: manohar.kamat @aerospace.gatech.edu, or the respective professional society webpages.

APRIL 4-10, 2000

10th INTERNATIONAL CONFERENCE ON HIGH TEMPERATURE MATERIALS CHEMISTRY
Aachen, Germany.

Information: Klaus Hilpert, Forschungszentrum Julich GmbH, Institut fur Werkstoffe der Energietechnik, Julich, Germany D-52425, (49) 2461 613280, Fax (49) 2461 613699, e-mail: k.hilpert@fz-juelich.de

APRIL 8-12, 2000

SPRING TECHNICAL CONFERENCE OF THE ASME INTERNAL COMBUSTION ENGINE DIVISION
San Antonio TX.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7054, Fax (212) 705-7143, http://www.asme.org

APRIL 10-14, 2000

10th INTERNATIONAL IUPAC CONFERENCE ON HIGH TEMPERATURE MATERIALS CHEMISTRY
Aachen, Germany.

Topics will Include:

- Synthesis, Properties, and Application of High Temperature Materials
- Vaporization, Molecules, and Clusters
- Interface Processes (Corrosion, Oxidation, Diffusion)
- Technical Processes and Devices at High Temperatures
- Thermodynamic and Kinetic Measurements, Modeling and Databases

Information: K. Hilpert, Forschungszentrum Julich GmbH, Institut fur Werkstoffe der Energietechnick (IWE 1), 52425 Julich, Germany, (49) 2461 61 3280, Fax (49) 2461 61 3699, e-mail: k.hilpert@fz-juelich.de, http://www.fz-juelich.de/oea/termine.html

APRIL 10-14, 2000

3rd INTERNATIONAL SEMINAR IN FIRE AND EXPLOSION HAZARDS
Lake Windermere, UK.

Information: G. Makhviladze, Centre for Research in Fire and Explosion Studies, University of Central Lancashire, Preston PR1 2HE, UK, (01772) 893222, Fax (01772) 892916, e-mail: g.makhviladze@uclan.ac.uk, http://www.uclan.ac.uk/commerc/fire.htm

APRIL 11-13, 2000

GASIFICATION FOR THE FUTURE
Noordwijk, The Netherlands.

Information: J. Black, IChemE's Conference Department, 165-189 Railway Terrace, Rugby, Warwickshire CV21 3HQ, UK, (44) 1788-578214, Fax (44) 1788-577182, e-mail: jblack@icheme.org.uk

APRIL 11-14, 2000

5th EUROPEAN CONFERENCE ON INDUSTRIAL FURNACES AND BOILERS
Porto, Portugal.

Information: INFUB c/o Albino Reis, Rua Gago Coutino, 185-187, 4435 Rio Tinto, Portugal, (2) 9734624/9730747, Fax (2) 9730746, e-mail: conference@infub.pt, http://www.infub.pt

APRIL 12-14, 2000

3C STEREO AND HOLOGRAPHIC PIV APPLICATION TO TURBULENCE MEASUREMENTS: EUROMECH COLLOQUIUM 411
Rouen, France.

Information: M. Trinite, CORIA-UMR 6614, Universite et INSA de Rouen, F-76821 Mont Saint Aignan Cedex, France, (33) 2-35-14-65-58, Fax (33) 2-35-70-83-84, e-mail: trinite@coria.fr

♦ APRIL 16-18, 2000

SPRING TECHNICAL MEETING OF THE CENTRAL STATES SECTION OF THE COMBUSTION INSTITUTE
Indianapolis IN.

Invited Papers Include:

- The Real Sequence of Processes to be Modeled in Diesel Engine Combustion
  P.F. Flynn, Cummins Engine Co., Inc.
- A Current Perspective on In-Cylinder Turbulent Thermal-Fluids Processes in Spark Ignited Reciprocating IC Engines
  D. Haworth, Pennsylvania State University
- Multidimensional Modeling of Reacting Flow in Stationary Combustors
  W.A. Fiveland, Combustion Engineering, Inc.
- Modeling of Gas-Turbine Combustors
  M.S. Anand, Rolls Royce Allison

Information: D.L. Reuss, General Motors R&D, 30500 Mound Road, Warren, MI 48090, (810) 986-0887, Fax (810) 986-0176, e-mail: dreuss@gmr.com
Deadline: Submit Abstract by January 4, 2000, 6-Page Paper by March 1, 2000. Abstracts of Poster Presentations by February 15, 2000.

APRIL 24-28, 2000

MATERIALS RESEARCH SOCIETY SPRING MEETING
San Francisco CA.

Information: Materials Research Society, Meetings Department, 506 Keystone Drive, Warrendale, PA 15086, (412) 779-3003, e-mail: info@mrs.org

♦ APRIL 26-30, 2000

2nd INTERNATIONAL CONFERENCE ON ATOMIC AND MOLECULAR DATA AND THEIR APPLICATIONS
Oxford UK.

Information: K. Berrington, e-mail: k.berrington@shu.ac.uk, http://physics.nist.gov/icamdata

APRIL 29-MAY 1, 2000

ANNUAL MEETING OF THE AMERICAN PHYSICAL SOCIETY
Long Beach CA.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

MAY 7-12, 2000

CLEO/QELS 2000
San Francisco CA.

Information: Meetings Department, American Physical Society, One Physics Ellipse, College Park, MD 20740, (301) 209-3286, http://www.osa.org/mtg_conf, http://physics.wm.edu/~cooke/dis/dis.html

MAY 8-11, 2000

ASME TURBO EXPO: LAND, SEA AND AIR
Munich, Germany.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (404) 847-0072 or (212) 591-7008, Fax (212) 705-7143, http://www.asme.org

♦ MAY 8-11, 2000

UNITED ENGINEERING CONFERENCE ON THE EFFECTS OF COAL QUALITY ON POWER PLANT PERFORMANCE: ASH PROBLEMS, MANAGEMENT AND SOLUTIONS
Park City UT.

Information: United Engineering Foundation, Meetings Department, Three Park Avenue, 27th Floor, New York, NY 10016, (212) 591-7836, Fax (212) 591-7441, e-mail: engfnd@aol.com, http://www.engfnd.org/engfnd/conf.html

MAY 14-19, 2000

197th MEETING OF THE ELECTROCHEMICAL SOCIETY
Toronto, Ontario, Canada.

Topics Include:
- General Session on Corrosion
- Plasma Processing
- 15th International Conference on Chemical Vapor Deposition
- Sensors for Energy Technologies

Information: http://www.electrochem.org/meetings

MAY 16-19, 2000

33rd MIDDLE ATLANTIC REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Newark DE.

Information: G.L. Trainor, DuPont Pharmaceuticals Co., P.O. Box 80353, Wilmington, DE 19880, (302) 695-3580, Fax (302) 695-8344, e-mail: trainogl@carbon.dmpc.com

MAY 17-19, 2000

32nd CENTRAL REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Covington KY.

Information: R. D'Alonzo, Procter & Gamble, Sharon Woods Technical Center, 11450 Grooms Road, Cincinnati, OH 45242, (513) 626-1977, Fax (513) 626-5145, e-mail: dalonzorp@pg.com

MAY 22-26, 2000

4th MINSK INTERNATIONAL HEAT AND MASS TRANSFER FORUM
Minsk, Belarus.

Information: I. Gurevich, Secretary of the MIF-IV Organizing Committee, A.V. Luikov Heat and Mass Transfer Institute, National Academy of Sciences of Belarus, 15, P. Brovka St., Minsk, 220072, Belarus, (375) 17.284-21-36, Fax (375) 17.232-25-13, e-mail: igur@hmti.ac.by, http://www.itmo.by/forum/forum7/index.html

JUNE 4-7, 2000

32nd GREAT LAKES REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Fargo ND.

Information: G.J. McCarthy, North Dakota State University, Department of Chemistry, Ladd Hall 104B, Fargo, ND 58105, (701) 231-7193, Fax (701) 231-8883, e-mail: gmccarth@prarie.nodak.edu

JUNE 4-8, 2000

TURN OF THE CENTURY IN ATOMIC SPECTROMETRY AND ELEMENT ANALYSIS: PAST, PRESENT AND FUTURE
Interlaken, Switzerland.

Information: G. Vujicic, SASP c/o IWM, Industriestr. 59, Glattbrugg, Switzerland CH-8152, (41) (0) 1 810 57 72, Fax (41) (0) 1 810 09 78, e-mail: gvujicic@swissonline.ch, http://www.sasp.ch/

JUNE 8-10, 2000

JOINT 55th NORTHWEST/16th ROCKY MOUNTAIN REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Idaho Falls ID.

Information: E.G. Meyer, 214 Arts & Sciences, University of Wyoming, Laramie, WY 82071, (307) 766-5445.

JUNE 11-15, 2000

SUMMER MEETING OF THE ASME FLUIDS ENGINEERING DIVISION
Boston MA.

Symposia will Include:
- Flows in Manufacturing Processes
- Numerical Developments in CFD
- Non-Invasive Measurements in Multiphase Flow
- Advances in Numerical Modeling of Aerodynamics and Hydrodynamics in Turbomachinery
- Erosion Processes
- Fluid Flow in Microsystems: Measurement, Analysis, and Applications
- Numerical Methods for Multiphase Flows
- Experimental and Numerical Flow Visualization and Laser Anemometry

Forums will be Held on the Following Topics:
- Finite Element Applications in Fluid Dynamics
- Turbulent Flows
- Laminar Flows

- High Speed Jet Flows
- Advances in Fluids Engineering Education
- CFD Applications in Automotive Flows
- Bifurcation, Instability, and Hysteresis in Fluid Flow
- Three-Dimensional Flows
- CFD Applications in Large Facilities
- Open Forum on Multiphase Flows
- Submicron Particle Flows
- Fluid Measurements and Instrumentation
- Fluid Machinery Forum
- Advances in Free Surface and Interface Fluid Dynamics
- Simulation of the Interaction of Transportation Vehicles with the Environment
- Forum on Developments in CFD Code Verification and Validation
- Cavitation and Multiphase Flow Forum

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 705-7037, Fax (212) 705-7143, http://www.asme.org

♦ JUNE 11-15, 2000

48th ASMS CONFERENCE ON MASS SPECTROMETRY AND ALLIED TOPICS
Long Beach CA.

Information: http://www.asms.org

♦ JUNE 14-17, 2000

DIVISION OF ATOMIC, MOLECULAR AND OPTICAL PHYSICS OF THE AMERICAN PHYSICAL SOCIETY
Storrs CT.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

JUNE 18-21, 2000

29th NORTHEAST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Storrs CT.

Information: G. Epling, University of Connecticut, 215 Glenbrook Road, Storrs, CT 06269, (860) 486-3214, Fax (860) 486-2981, e-mail: epling@nucleus.chem.uconn.edu

JUNE 18-22, 2000

ANNUAL MEETING OF THE AIR AND WASTE MANAGEMENT ASSOCIATION
Salt Lake City UT.

Information: Air and Waste Management Association, Member Services, One Gateway Center, Third Floor, Pittsburgh, PA 15222, (800) 270-3444 or (412) 232-3444, Fax (412) 232-3450, http://www.awma.org

JUNE 18-23, 2000

OPTICS IN COMPUTING
Quebec City, Quebec, Canada.

Information: Meetings Department, SPIE, P.O. Box 10, Bellingham, WA 98227, (360) 676-3290, Fax (360) 647-1445, e-mail: spie@spie.org, http://www.spie.org

JUNE 19-20, 2000

CEC/SAE FUELS AND LUBRICANTS SPRING MEETING AND EXPOSITION
Le Palais des Congress, Paris, France.

Information: Society of Automotive Engineers, Inc., 400 Commonwealth Drive, Warrendale, PA 15096, (724) 776-4841, Fax (724) 776-5760, e-mail: meetings@sae.org, http://www.sae.org

♦ JUNE 19-22, 2000

21st AIAA ADVANCED MEASUREMENT TECHNOLOGY AND GROUND TESTING CONFERENCE: FLUIDS 2000 AND EXHIBIT: 31st AIAA PLASMADYNAMICS AND LASERS CONFERENCE: 34th AIAA THERMOPHYSICS CONFERENCE
Denver CO.

Information: J.A. Morrow, Department of Aeronautics, United States Air Force Academy, 2354 Fairchild Drive, #6H22, U.S. Air Force Academy, CO 80840, (719) 333-3434, Fax (719) 333-4813, e-mail: MorrowJA.dfan@usafa.af.mil, or http://www.aiaa.org

JULY 1-7, 2000

WORLDWIDE RENEWABLE ENERGY CONGRESS
Brighton UK.

Information: A. Sayrigh, 147 Hilmanton, Lower Earley, Reading RG6 4HN, UK.

JULY 10-13, 2000

10th INTERNATIONAL SYMPOSIUM ON APPLICATIONS OF LASER TECHNIQUES TO FLUID MECHANICS
Lisbon, Portugal.

Information: G. Pereira, Mechanical Engineering Department, Instituto Superior Tecnico, 1049-001 Lisboa, Portugal, Fax (351) 1-849-6156, e-mail: llaser@dem.ist.utl.pt, http://in3.dem.ist.utl.pt/lisboa-laser

♦ JULY 16-19, 2000

36th AIAA/ASME/SAE/ASEE JOINT PROPULSION CONFERENCE AND EXHIBIT ON PROPULSION: THE KEY TO EXPLORING NEW WORLDS
Huntsville AL.

Information: B. Noblitt, Conference General Chair, TRW, Suite 1231, 303 Williams Avenue, Huntsville, AL 35801, (256) 533-3714, Fax (256) 533-0137, e-mail: bobby.noblitt@trw.com, or http://www.aiaa.org/calendar

♦ JULY 23-26, 2000

ASME INTERNATIONAL JOINT POWER GENERATION CONFERENCE AND EXPOSITION
Miami Beach FL.

Information: N.A. Moussa, BlazeTech Corporation, 24 Thorndike Street, Cambridge, MA 02141, (617) 661-0700, Fax (617) 661-9242, amoussa@blazetech.com, or http://www.asme.org/conf/

JULY 23-28, 2000

ENERGEX 2000: 8th INTERNATIONAL ENERGY FORUM
Las Vegas NV.

Topics will Include:

- Renewable Energies
- Clean Coal Technologies
- Fossil Fuels
- Energy and Economics
- Climatic Change
- International Law
- General Topics
- International Reports
- Nuclear Energy
- Architecture

Information: P. Catania, Faculty of Engineering, University of Regina, Regina, SK S4S 0A2, Canada, (306) 585-4363, Fax (306) 585-4855, e-mail: peter.catania@uregina.ca, http://www2.regina.ism.ca/ief/index/htm or http://www.energysource.com/ief/updates/

JULY 24-28, 2000

35th INTERSOCIETY ENERGY CONVERSION ENGINEERING CONFERENCE
Las Vegas NV.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7008, Fax (212) 705-7143, http://www.asme.org

JULY 30-AUGUST 4, 2000

SPIE ANNUAL MEETING
San Diego CA.

Information: Meetings Department, SPIE, P.O. Box 10, Bellingham, WA 98227, (360) 676-3290, Fax (360) 647-1445, e-mail: spie@spie.org, http://www.spie.org

JULY 30-AUGUST 4, 2000

28th INTERNATIONAL SYMPOSIUM ON COMBUSTION
Edinburgh, Scotland.

Information: S.S. Terpack, The Combustion Institute, 5001 Baum Boulevard, Suite 635, Pittsburgh, PA 15212, (412) 687-1366, Fax (412) 687-0340, e-mail: combust@telerama.lm.com

AUGUST 1-5, 2000

35th IECEC Intersociety Energy Conversion Engineering Conference
Las Vegas NV.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7008, Fax (212) 705-7143, http://www.asme.org

AUGUST 13-18, 2000

Turbine 2000, International Symposium on Heat Transfer in Gas Turbine Systems
Izmir, Turkey.

Information: R.J. Goldstein, Conference Chair, Department of Mechanical Engineering, University of Minnesota, Minneapolis, MN 55455, (612) 625-5552, Fax (612) 625-3434, e-mail: rjgumn@mailbox.mail.umn.edu, http://ichmt.me.metu.edu.tr
Deadline: Abstracts Due by February 29, 2000.

♦ AUGUST 14-17, 2000

18th AIAA Applied Aerodynamics Conference
Denver CO.

Information: N.E. Suhs, Applied Aerodynamic Technical Program Chair, Naval Air Systems Command, Building 2187, Unit 5, Suite 1390A, 48110 Shaw Road, Patuxent River, MD 20670, (301) 342-0311, Fax (301) 342-8585, e-mail: suhsne@navair.navy.mil, or http://www.aiaa.org/calendar
Deadline: Abstract by January 3, 2000

AUGUST 20-24, 2000

220th National Meeting of the American Chemical Society
Washington DC.

Division of Fuel Chemistry:

- 1990 Clean Air Act Amendments: A 10-Year Assessment
  J.J. Helble, University of Connecticut, Department of Chemical Engineering, U-222, Storrs, CT 06269, (860) 486-4602, Fax (860) 486-2959, e-mail: helble@eng2.uconn.edu
- Inorganics in Fossil Fuels, Waste Materials, and Biomass: Characterization, Combustion Behavior, and Environmental Issues
  C.L. Senior, Physical Sciences, Inc., 20 New England Business Center, Andover, MA 01810, (978) 689-0003, Fax (978) 689-3232, e-mail: senior@psicorp.com
- Waste Material Recycling for Energy and Other Applications
  S.V. Pisupati, Fuel Science Program, Pennsylvania State University, 404 Academic Projects Building, University Park, PA 16802, (814) 865-0874, Fax (814) 863-8892, e-mail: sxp17@psu.edu
- Fossil Fuels and Global Climate/CO_2 Abatement
  R. Warzinski, USDOE/FETC, Box 10940, Building 83-324, Pittsburgh, PA 15236, (412) 892-5863, e-mail: warzinsk@fetc.doe.gov
- Production of Fuels and Chemicals from Synthesis Gas
  D.B. Dadyburjor, Department of Chemical Engineering, P.O. Box 6102, West Virginia University, Morgantown, WV 26506, (304) 293-2111 ext 2411, Fax (304) 293-4139, e-mail: dadyburjor@cemr.wvu.edu
- Solid Fuel Chemistry
- Chemistry of Liquid and Gaseous Fuels

F. Huggins, South Limestone St., Suite 111, University of Kentucky, Lexington, KY 40506, (606) 257-4045, Fax (606) 257-7215, e-mail: fhuggins@engr.uky.edu

Division of Petroleum Chemistry:

- Emission Control in Petroleum Processing
  P. O'Connor, U.S. Ozkan, Department of Chemical Engineering, Ohio State University, 140 W. 19th Avenue, Columbus, OH 43210, (614) 292-6623, Fax (614) 292-3769, e-mail: ozkan.1@osu.edu
- Structure of Jet Fuels VI
  W.E. Harrison, Department of the Air Force, WL/POSF, Building 490, Area B, 1790 Loop Road N., Wright-Patterson AFB, OH 45433, (937) 255-6601, Fax (937) 255-1125, e-mail: harriswe@wl.pafb.af.mil

Division of Physical Chemistry:

- Chemistry Under Extreme Conditions
  R. Morris, AFRL/VSBP, 29 Randolph Rd., Hanscom AFB, MA 01731, (781) 377-8758, Fax (781) 377-5088, e-mail: morris@plh.af.mil
- Very Low Temperature Spectroscopy and Dynamics
  W. Stwalley, Department of Physics, University of Connecticut, 2152 Hillside Road, Storrs, CT 06269, (860) 486-4924, Fax (860) 486-3346, e-mail: stwalley@uconnvm.uconn.edu

Information: From the Individual Chairpersons or from the Meetings Department, American Chemical Society, 1155 - 16th Street, NW, Washington, DC 20036, (202) 872-4396, Fax (202) 872-6128, e-mail: natlmtgs@acs.org

AUGUST 20-22, 2000

34th ASME National Heat Transfer Conference
Pittsburgh PA.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7795, Fax (212) 705-7143, http://www.asme.org

AUGUST 22-25, 2000

9th International (Millennium) Symposium on Flow Visualization
Edinburgh, Scotland.

Information: I. Grant, Heriot-Watt University, Edinburgh, Scotland, EH10 5PJ, UK, (44) 1314478800, Fax (44) 1314478660, e-mail: 9misfv@ode-web.demon.co.uk, Web Site: http://www.ode-web.demon.co.uk/9misfv
Deadline: Abstract Template should be Downloaded from the Web. 4 Pages or Less to be Submitted by December 12, 1999. Final Manuscripts Due May 15, 2000.

AUGUST 26-30, 2000

15th Europhysics Conference on Atomic and Molecular Physics of Ionized Gases
Miskolc-Lillafured, Hungary.

Information: Z. Donko, c/o Eotvos Lorand Physical Society, H-1371 Budapest, P.O. Box 433, Hungary, e-mail: escampig@elft.mtesz.hu, http://elft.mtesz.hu/escampig2000

AUGUST 27-SEPTEMBER 1, 2000

25th European Congress on Molecular Spectroscopy

Coimbra, Portugal.

Information: R. Fausto, Department of Chemistry, University of Coimbra, Coimbra, Portugal P-3049, (351) 39-852080, Fax (351) 39-827703, e-mail: rfausto@gemini.ci.uc.pt, http://qui.uc.pt/~rfausto/eucmos_xxv

SEPTEMBER 3-7, 2000

16th INTERNATIONAL CONFERENCE ON HIGH RESOLUTION MOLECULAR SPECTROSCOPY
Prague, Czech Republic.

Information: S. Urban, UFCH JH Academy of Sciences of the Czech Republic, Dolejskova 3, Prague, Czech Republic, CZ-18223, (420) 2-6605-3635, Fax (420) 2-858-2307, e-mail: praha2k@jh-inst.cas.cz, http://www.chem.uni-wuppertal.de/conference/

SEPTEMBER 10-13, 2000

3rd EUROPEAN THERMAL SCIENCES CONFERENCE
Heidelberg, Germany.

Information: E. Hahne, Institut fur Thermodynamik und Warmetechnik, Pfaffenwaldring 6, 70550 Stuttgart, Germany, 49 (0) 711-685-3536, Fax 49 (0) 711-685-3503, e-mail: pm@itw.uni-stuttgart.de

SEPTEMBER 10-15, 2000

CONFERENCE ON LASERS AND ELECTRO-OPTICS (CLEO) AND THE INTERNATIONAL QUANTUM ELECTRONICS CONFERENCE (IQEC)
Nice, France.

Information: Optical Society of America, Meetings Department, 2010 Massachusetts Ave NW, Washington, DC 20036, (202) 223-0920, e-mail: confserv@osa.org

♦ SEPTEMBER 13-16, 2000

2nd INTERNATIONAL CONFERENCE ON INORGANIC MATERIALS
Santa Barbara CA.

Information: Sarah Wilkinson, Conference Secretariat, Elsevier Science Ltd., The Boulevard, Langford Lane, Kidlington, Oxford, UK OX5 1GB, 44(0) 1865 843691, Fax 44(0) 1865 843658, e-mail: sm.wilkinson@elsevier.co.uk, http://www.elsevier.com/locate/im2000

♦ SEPTEMBER 18-20, 2000

13th International Symposium on Gas Flow and Chemical Lasers and High Power Laser Conference
Florence, Italy.

Information: C. Pescucci, Fax 39(0) 55-233-7755, e-mail: gcl-hpl@ino.it, www.ino.it/GCL-HPL or www.es.titech.ac.jp/~kkasuya/gcl-web/index.html

SEPTEMBER 19-21, 2000

The Hydrogen Energy Forum 2000
Munich, Germany.

Information: The Future Energies Forum, "Forum fur Zukunftsenergien", Godesberger Allee 90, D-53175 Bonn, Germany, Fax 49(0) 228-959 56-50, e-mail: energie.forum@t-online.de

SEPTEMBER 22-30, 2000

27th Annual Conference of the Federation of Analytical Chemistry and Spectroscopy Societies
Nashville TN.

Information: Division of Analytical Chemistry, FACSS, (505) 820-1648, Fax (505) 989-1073, Web Site: http://FACSS.org/info.html

SEPTEMBER 23-26, 2000

ASME Fall Technical Conference of the Internal Combustion Engine Division
Peoria IL.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7054, Fax (212) 705-7143, http://www.asme.org

♦ SEPTEMBER 24-26, 2000

1st Romanian International Conference on Analytical Chemistry
Brasov, Romania.

Information: G.L. Radu, University of Bucharest, Faculty of Chemistry, 4-12, Elisabeta Blvd., Bucharest, Romania 703461, 40(1) 220 77 80/220 79 09, Fax 40(1) 220 76 95, e-mail: lucian@ibd.dbio.ro

♦ OCTOBER 2-5, 2000

ICALEO 2000, International Conference on Applied Laser Applications and Electrooptics
Dearborn MI.

Information: E. Cohen, Laser Institute of America, (800) 345-2737 or (407) 380-1553, Fax (407) 380-5588, http://www.laserinstitute.org

OCTOBER 8-11, 2000

GASIFICATION TECHNOLOGIES CONFERENCE
San Francisco CA.

Information: M. Samoulides, (650) 855-2127, or Electric Power Research Institute, 1412 Hillview Avenue, Palo Alto, CA 94304, (650) 855-2599, http://www.epri.com

OCTOBER 16-19, 2000

INTERNATIONAL FUEL AND LUBRICANTS FALL MEETING AND EXPOSITION OF THE SOCIETY OF AUTOMOTIVE ENGINEERS
Baltimore MD.

Information: Society of Automotive Engineers, Inc., 400 Commonwealth Drive, Warrendale, PA 15096, (724) 776-4841, Fax (724) 776-5760, e-mail: meetings@sae.org, Web Site: http://www.sae.org

OCTOBER 22-27, 2000

198th NATIONAL MEETING OF THE ELECTROCHEMICAL SOCIETY
Phoenix AZ.

Information: The Electrochemical Society, Inc., Meetings Department, 10 South Main Street, Pennington, NJ 08534, (609) 737-1902, Fax (609) 737-2743, e-mail: ecs@electrochem.org, http://www.electrochem.org/meetings/198/meet.html

♦ OCTOBER 24-27, 2000

53rd ANNUAL GASEOUS ELECTRONICS CONFERENCE OF THE AMERICAN PHYSICAL SOCIETY
Houston TX.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

OCTOBER 25-28, 2000

35th MIDWEST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
St Louis MO.

Information: C.D. Spilling, Department of Chemistry, University of Missouri, St. Louis, 80001 Natural Bridge Road, St. Louis, MO 63121 (314) 516-5313, Fax (314) 553-5342, e-mail: cspill@umsl.edu

OCTOBER 29-NOVEMBER 3, 2000

EASTERN ANALYTICAL SYMPOSIUM OF THE AMERICAN CHEMICAL SOCIETY
Atlantic City NJ.

Information: S. Gold, Eastern Analytical Symposium, P.O. Box 633, Montchanin, DE 19710 (302) 738-6218, Fax (302) 738-5275, http://www.eas.org

♦ NOVEMBER 2-4, 2000

SOUTHEAST SECTION MEETING OF THE AMERICAN PHYSICAL SOCIETY
Starkville MS.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

♦ NOVEMBER 3-8, 2000

PHOTONICS EAST
Boston MA.

Information: Meetings Department, SPIE, P.O. Box 10, Bellingham, WA 98227, (360) 676-3290, Fax (360) 647-1445, e-mail: spie@spie.org, http://www.spie.org

NOVEMBER 5-10, 2000

ASME INTERNATIONAL MECHANICAL ENGINEERING CONFERENCE AND EXHIBITION
Orlando FL.

Symposia will Include:

- Symposium on Multiphase Flow in Biomedical Applications and Processes
- Dispersed Flows in Combustion, Incineration, and Propulsion Systems
- Application of Microfabrication to Fluid Mechanics

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 705-7037, Fax (212) 705-7143, http://www.asme.org

NOVEMBER 5-10, 2000

INTERNATIONAL SYMPOSIUM ON MULTIPHASE FLOW AND TRANSPORT PHENOMENA
Antalya, Turkey.

Topics will Include:

- Modeling of Multiphase Systems
- Transport Phenomena in Multiphase Systems
- Separation Phenomena, Processes and Equipment
- Measurement and Instrumentation
- Characteristic and Effective Properties of Multiphase Systems
- Bio-Aerosols and Bio-Systems
- Surface and Interfacial Phenomena
- Pollution Control Technology
- Clean Room Technology
- Multiphase Systems Applications
- Scaling Laws for Two-Phase Flow Phenomena
- Scaling Laws for Multiphase Flow

Information: D.M. Maron, Center for Technological Education Holon, POB 305, Holon 58102, Israel, (972) 3-502 6501, Fax (972) 3-502 6510, e-mail: barad_r@barley.cteh.ac.il, http://ichmt.me.metu.edu.tr/upcoming-meetings/MFTP-00/announce.html

♦ NOVEMBER 5-10, 2000

UNITED ENGINEERING FOUNDATION CONFERENCE ON LEAN COMBUSTION TECHNOLOGY AND CONTROL
Santa Fe NM.

Information: United Engineering Foundation, Meetings Department, Three Park Avenue, 27th Floor, New York, NY 10016, (212) 591-7836, Fax (212) 591-7441, e-mail: engfnd@aol.com http://www.engfnd.org/engfnd/conf.html, or from D. Dunn-Rankin, University of California at Irvine, CA, or R.K. Cheng, Lawrence Berkeley National Laboratory.

♦ NOVEMBER 12-17, 2000

ANNUAL MEETING OF THE AMERICAN INSTITUTE OF CHEMICAL ENGINEERS
Los Angeles, CA.

Information: Meetings Department, American Institute of Chemical Engineers, United Engineering Center, 3 Park Avenue, New York, NY 10016, (212) 591-7325, Fax (212) 591-8894, e-mail: meetmail@aiche.org, http://www.aiche.org

NOVEMBER 13-18, 2000

EASTERN ANALYTICAL SYMPOSIUM OF THE AMERICAN CHEMICAL SOCIETY
Somerset NJ.

Information: S. Gold, Eastern Analytical Symposium, P.O. Box 633, Montchanin, DE 19710, (302) 738-6218, Fax (302) 738-5275, Web Site: http://www.eas.org

♦ NOVEMBER 19-21, 2000

DIVISION OF FLUID DYNAMICS MEETING OF THE AMERICAN PHYSICAL SOCIETY
Washington DC.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

♦ NOVEMBER 27-DECEMBER 1, 2000

FALL MEETING OF THE MATERIALS RESEARCH SOCIETY
Boston MA.

Information: Materials Research Society, Meetings Department, 506 Keystone Drive, Warrendale, PA 15086, (724) 779-3003, Fax (724) 779-8313, http://www.mrs.org

DECEMBER 6-8, 2000

JOINT 52nd SOUTHEAST/56th SOUTHWEST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
New Orleans LA.

Information: A. Pepperman, SRRC, USDA-ARS, 1100 Robert E. Lee Boulevard, New Orleans, LA 70179, (208) 286-4510, Fax (208) 286-4367, e-mail: abpep@nola.srrc.usda.gov

DECEMBER 14-19, 2000

INTERNATIONAL CHEMICAL CONGRESS OF PACIFIC BASIN SOCIETIES
Honolulu HI.

Information: Meetings Department, American Chemical Society, 1155 - 16th Street, NW, Washington, DC 20036, (202) 872-4396, Fax (202) 872-6128, e-mail: natlmtgs@acs.org

MARCH 4-8, 2001

THE PITTSBURGH CONFERENCE, PITTCON 2001
New Orleans LA.

Information: The Pittsburgh Conference, 300 Penn Center Boulevard, Suite 332, Pittsburgh, PA 15235, (412) 825-3220, Fax (412) 825-3224, e-mail: pittconinfo@pittcon.org, http://www.pittcon.org/

MARCH 12-16, 2001

ANNUAL MARCH MEETING OF THE AMERICAN PHYSICAL SOCIETY
Seattle WA.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

MARCH 25-30, 2001

199th NATIONAL MEETING OF THE ELECTROCHEMICAL SOCIETY
Washington DC.

Information: The Electrochemical Society, Inc., Meetings Department, 10 South Main Street, Pennington, NJ 08534, (609) 737-1902, Fax (609) 737-2743, e-mail: ecs@electrochem.org, http://www.electrochem.org/meetings/199/meet.html

APRIL 1-5, 2001

221st NATIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
San Diego CA.

Division of Fuel Chemistry:

- CO_2 Capture and/or Utilization Reaction Mechanisms in Fuel Processing
  P.F Britt, Chemistry Division, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN 37831, (423) 574-5029, Fax (423) 576-5235, e-mail: brittpf@ornl.gov
- Coal Bed Methane
  P.C. Thakur, Consol Inc., R&D, 1027 Little Indian Creek Road, Morgantown, WV 26501, (304) 983-3207, Fax (304) 983-3209, e-mail: promodthakur@consolcoal.com
- Nitrogen Chemistry in Coal Utilization
  M.A. Wojtowicz, Advanced Fuel Research Inc., 87 Church Street, East Hartford, CT 06108, (860) 528-9806 ext 142, Fax (860) 528-0648, e-mail: marek@afrinc.com
- Hydrogen Energy
  R. Khan, Texaco Inc., P.O. Box 509, Beacon, NY 12508, (914) 838-7639, Fax (914) 838-7102
- Argonne National Lab Premium Coal Sample Database
  K. Vorres, 27 Windward Circle, Willowbrook, IL 60514, (630) 325-0931 [between Nov. 11 and April 15: 3432 North Applewood, Tucson, AZ 85712-5478, (520) 322-5256], e-mail: ksvorres@flash.net
- Carbon Products for Environmental Applications

A. Lizzio, Illinois State Geological Survey, 615 East Peabody Drive, Champaign, IL 61801, (217) 244-4985, Fax (217) 333-8566, e-mail: lizzio@geoserv.isgs.uiuc.edu

♦ APRIL 16-20, 2001

SPRING MEETING OF THE MATERIALS RESEARCH SOCIETY
San Francisco CA.

Information: Materials Research Society, Meetings Department, 506 Keystone Drive, Warrendale, PA 15086, (724) 779-3003, Fax (724) 779-8313, http://www.mrs.org

APRIL 23-27, 2001

APRIL NATIONAL MEETING OF THE AMERICAN PHYSICAL SOCIETY
Washington DC.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

MAY 6-11, 2001

CLEO/QELS 2001
Baltimore MD.

Information: Optical Society of America, Meetings Department, 2010 Massachusetts Ave NW, Washington, DC 20036, (202) 223-0920, e-mail: confserv@osa.org, http://www.osa.org/mtg_conf

MAY 20-25, 2001

FLUIDIZATION X
Beijing, China.

Information: United Engineering Foundation, Meetings Department, Three Park Avenue, 27th Floor, New York, NY 10016, (212) 591-7836, Fax (212) 591-7441, http://www.engfnd.org/engfnd/conf.html

MAY 20-25, 2001

2nd INTERNATIONAL SYMPOSIUM ON ADVANCES IN COMPUTATIONAL HEAT TRANSFER
Cairns, Australia.

Information: F. Arinc, Secretary-General, ICHMT, Mechanical Engineering Department, Middle East Technical University, 06531 Ankara, Turkey, (90) 312-210-1429, Fax (90) 312-210-1331, arinc@metu.edu.tr, http://ichmt.me.metu.edu.tr

MAY 30-JUNE 1, 2001

35th Middle Atlantic Regional Meeting of the American Chemical Society
Baltimore MD.

Information: L.J. Boucher, Towson University, Department of Chemistry, 8000 York Road, Towson, MD 21252-0001, (410) 830-3057, Fax (410) 830-4265, e-mail: lboucher@towson.edu

JUNE 13-15, 2001

Joint 33rd Central/33rd Great Lakes Regional Meeting of the American Chemical Society
Grand Rapids MI.

Information: R.J. McCabe, Parke-Davis, 188 Howard Avenue, Holland, MI 49423, (616) 392-2375 ext 2386, Fax (616) 392-8916, e-mail: Richard.McCabe@wl.com

JUNE 13-16, 2001

56th Northwest Regional Meeting of the American Chemical Society
Seattle WA.

Information: S. Jackels, Department of Chemistry, Seattle University, 900 Broadway, Seattle, WA 98122, (206) 296-5946, Fax (206) 296-5786, e-mail: sjackels@seattleu.edu

JUNE 24-28, 2001

Annual Meeting of the Air and Waste Management Association
Orlando FL.

Information: Air and Waste Management Association, Member Services, One Gateway Center, Third Floor, Pittsburgh, PA 15222, (800) 270-3444 or (412) 232-3444, Fax (412) 232-3450, http://www.awma.org

JULY 9-11, 2001

Combustion Chemistry: Elementary Reactions to Macroscopic Processes: Faraday Discussion Number 119
Leeds, UK.

Joint Meeting with the British Section of the Combustion Institute.
Information: M. Pilling, School of Chemistry, University of Leeds, Leeds UK, e-mail: m.j.pilling@chem.leeds.ac.uk, http://www.chem.leeds.ac.uk

AUGUST 20-24, 2001

13th International Conference on Fourier Transform Spectroscopy
Turku, Finland.

Information: M. Hotokka, Department of Physical Chemistry, Abo Akademi University, FIN-20500 Turku, Finland, (358) 2-265-4295, Fax (358) 2-265-4706, e-mail: icofts@abo.fi, http://www.abo.fi/icofts

AUGUST 26-30, 2001

222nd National Meeting of the American Chemical Society
Chicago IL.

Information: Meetings Department, American Chemical Society, 1155 - 16th Street, NW, Washington, DC 20036, (202) 872-4396, Fax (202) 872-6128, e-mail: natlmtgs@acs.org

SEPTEMBER 2-7, 2001

200th National Meeting of the Electrochemical Society and the 52nd Meeting of the International Society of Electrochemistry
San Francisco CA.

Information: The Electrochemical Society, Inc., Meetings Department, 10 South Main Street, Pennington, NJ 08534, (609) 737-1902, Fax (609) 737-2743, e-mail: ecs@electrochem.org, http://www.electrochem.org/meetings/198/meet.html

SEPTEMBER 23-27, 2001

52nd Southeast Regional Meeting of the American Chemical Society
Savannah GA.

Information: G. Novotnak, Kemira Pigments, 104 Carlton Road, Savannah, GA 31410, (912) 652-1290, Fax (912) 897-1163, e-mail: george.novotnak@kemira.com

♦ SEPTEMBER 23-27, 2001

6th World Congress of Chemical Engineering: A New Century of Chemical Engineering
Melbourne, Australia.

Information: Meetings Department, American Institute of Chemical Engineers, United Engineering Center, 3 Park Avenue, New York, NY 10016, (212) 591-7325 or (800) 242-4363, Fax (212) 591-8894, e-mail: meetmail@aiche.org, http://www.aiche.org

OCTOBER 5-12, 2001

28th Annual Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies
Detroit MI.

Information: C. Lilly, Federation of Analytical Chemistry and Spectroscopy Societies, 1201 Don Diego Ave., Santa Fe, NM 87505, (505) 820-1648, Fax (505) 989-1073, e-mail: jsjoberg@trail.com, http://facss.org/info.html

OCTOBER 10-13, 2001

36th MIDWEST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Lincoln NE.

Information: D. Berkowitz, Department of Chemistry, University of Nebraska, Lincoln, NE 68588-0304, (402) 472-2738, Fax (402) 472-9402, e-mail: dbb@unlinfo.edu

OCTOBER 14-19, 2001

INTERNATIONAL SYMPOSIUM ON VISUALIZATION AND IMAGING IN TRANSPORT
Antalya, Turkey.

Information: F. Arinc, Secretary-General, ICHMT, Mechanical Engineering Department, Middle East Technical University, 06531 Ankara, Turkey, (90) 312-210-1429, Fax (90) 312-210-1331, arinc@metu.edu.tr, http://ichmt.me.metu.edu.tr

OCTOBER 16-19, 2001

57th SOUTHWEST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
San Antonio TX.

Information: S.T. Weintraub, Department of Biochemistry, University of Texas Health Science Center, 7703 Floyd Curl Drive, San Antonio, TX 78284, (210) 567-4043, Fax (210) 567-5524, e-mail: weintraub@uthscsa.edu

OCTOBER 23-26, 2001

36th WESTERN REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Ventura CA.

Information: R.W. Hurst, 9 Faculty Court, Thousand Oaks, CA 91360, (805) 492-7764, Fax (805) 241-7149, e-mail: Alarwh@aol.com

♦ NOVEMBER 26-30, 2001

FALL MEETING OF THE MATERIALS RESEARCH SOCIETY
Boston MA.

Information: Materials Research Society, Meetings Department, 506 Keystone Drive, Warrendale, PA 15086, (724) 779-3003, Fax (724) 779-8313, e-mail: info@mrs.org

CURRENT BIBLIOGRAPHY RELEVANT TO FUNDAMENTAL COMBUSTION

July 1999

Keith Schofield, ChemData Research, P.O. Box 40481
Santa Barbara, CA 93140, (805) 966-7768, Fax (805) 893-8797
e-mail: combust@mrl.ucsb.edu
http://www.ca.sandia.gov/CRF/Publications/CRB/CRB.html

1. FUELS/SYNFUELS - GENERAL

81709.	Penner, S.S., "United States Energy Supplies for the 21st Century," *Energy* 23, 71-78 (1998).	Energy Supplies US Needs Assessment
81710.	Mirabile, A., "Water in Oil Fuel Emulsion: A Reality to Reduce NO_x and Particulate Emissions and to Increase Boiler and Process Furnaces Availability/Efficiency," pp. 319-329 in *Combustion and Emissions Control II*, Proceedings of the Institute of Energy's *2nd International Conference*, Held in London UK, December 1995, Institute of Energy, London UK (1995).	Oil/H_2O Emulsion Fuel Viable Technology NO_x,SO_x Emissions
81711.	Jones, A.R., "The Commercial Combustion of Orimulsion™," pp. 318-339 in *Combustion and Emissions Control. III*, A Collection of 23 Papers, 350 pp., Institute of Energy, London UK (1997).	Emulsified Bitumen Fuel Combustion Trials Performance
(81729)	Co-firing Performance, FBC, Boilers	Coal/Biomass
(81754)	Co-firing Performance, NO Emissions, Ash Content	Coal/Biomass Coal/Sludge
(81730)	Co-firing, FBC, Design Changes, Performance, Emissions	Coal/Straw
81712.	Klass, D.L., *"Biomass for Renewable Energy, Fuels and Chemicals,"* 651 pp., Academic Press, San Diego CA (1998).	Biomass Energy Potential Combustion Pyrolysis Gasification Liquefaction Monograph
81713.	Steinfeld, A., M. Brack, A. Meier, A. Weidenkaff and D. Wuillemin, "A Solar Chemical Reactor for Co-production of Zinc and Synthesis Gas," *Energy* 23, 803-814 (1998).	Syn Gas Formation ZnO+CH_4 Solar Reactor Zn,CO,H_2 Products Efficiency

2. LIQUEFACTION/GASIFICATION

81714.	Lee, J.M., Y.J. Kim, W.J. Lee and S.D. Kim, "Coal Gasification Kinetics Derived from Pyrolysis in a Fluidized Bed Reactor," *Energy* 23, 475-488 (1998).	Gasification Coal FB Reactor Product Gases
81715.	Lee, J.M., Y.J. Kim and S.D. Kim, "Catalytic Coal Gasification in an Internally Circulating Fluidized Bed Reactor with Draft Tube," *Appl. Thermal Eng.* 18, 1013-1024 (1998).	Gasification Coal Catalytic FB Reactor
81716.	Dervisoglu, M., and O. Hortacsu, "An Experimental Study of Coal Gasification," *Energy* 23, 1073-1076 (1998).	Gasification Coal Fuel Heating Value Parameters
81717.	Norman, J.S., M. Pourkashanian and A. Williams, "The Formation of Ammonia in IGCC Gasifiers and Its Control," pp. 109-118 in *Combustion and Emissions Control II*, Proceedings of the Institute of Energy's *2nd International Conference*, Held in London UK, December 1995, Institute of Energy, London UK (1995).	Gasification Coal NH_3,HCN Formation/Control Kinetic Model
81718.	Griffiths, A.J., C.S. Avennel and N. Syred, "Flaming Pyrolysis: A Novel Approach for the Production of Biofuels," pp. 277-292 in *Combustion and Emissions Control. III*, A Collection of 23 Papers, 350 pp., Institute of Energy, London UK (1997).	Gasification Wastes Flaming Pyrolysis Method
81719.	Wallman, P.H., C.B. Thorsness and J.D. Winter, "Hydrogen Production from Wastes," *Energy* 23, 271-278 (1998).	Gasification Pyrolyzer Wastes Synfuel,H_2 Formation
(81712)	Biomass, Energy Potential, Monograph	Gasification Liquefaction
81720.	Hoppesteyn, P.D.J., W. de Jong, J. Andries and K.R.G. Hein, "Combustion of Biomass-Derived Low Calorific Value Fuel Gas," pp. 293-303 in *Combustion and Emissions Control. III*, A Collection of 23 Papers, 350 pp., Institute of Energy, London UK (1997).	Gasification Biomass Low Calorie Fuel Combustion
81721.	Wolf, D., "High Yields of Methanol from Methane by C-H Bond Activation at Low Temperatures," *Angew. Chem. Int. Ed. Engl.* 37, 3351-3353 (1998).	Partial Oxidation CH_4/CH_3OH CH_4/H_2SO_4(l)/Pt Efficient Method
81722.	Bodke, A.S., D.A. Olschki, L.D. Schmidt and E. Ranzi, "High Selectivities to Ethylene by Partial Oxidation of Ethane," *Science* 285, 712-715 (1999).	Partial Oxidation $C_2H_6/H_2/O_2$/Pt High Yields C_2H_4

3. BURNERS

(See also Section 21 for Burner Emissions and Incinerator Performance)

81723.	Yuan, J., and I. Naruse, "Modeling of Combustion Characteristics and NO_x Emission in Highly Preheated and Diluted Air Combustion," *Int. J. Energy Res.* 22, 1217-1234 (1998).	Regenerative Furnace Highly Preheated Diluted Air NO_x Emissions
81724.	Park, B.-S., D.-H. Chung, W.-B. Kim and Y. Kim, "A Study on the Design of Recuperative Burner," *Int. J. Energy Res.* 22, 209-220 (1998).	Recuperative Burners Design Efficiencies
81725.	Voyages, C.M., G. Papadakis and G. Bergeles, "Slag Formation and Motion in Pressurized Pulverized Coal Combustors," pp. 209-218 in *Combustion and Emissions Control II*, Proceedings of the Institute of Energy's *2nd International Conference*, Held in London UK, December 1995, Institute of Energy, London UK (1995).	Pulverized Coal Furnace Ash Particles Slag Formation Wall Creep Model
81726.	Huilin, L., B. Rushan, Y. Lidan, Z. Guangbo and T. Xiu, "Numerical Computation of a Circulating Fluidized Bed Combustor," *Int. J. Energy Res.* 22, 1351-1364 (1998).	FBC Circulating Numerical Model
81727.	Peirano, E., and B. Leckner, "Fundamentals of Turbulent Gas-Solid Flows Applied to Circulating Fluidized Bed Combustion," *Prog. Energy Combust. Sci.* 24, 259-296 (1998).	FBC Circulating Gas/Solid Flow Modeling
81728.	Leckner, B., "Fluidized Bed Combustion: Mixing and Pollutant Limitation," *Prog. Energy Combust. Sci.* 24, 31-61 (1998).	FBC Full Scale Mixing Aspects NO_x ,SO_2 Effects
81729.	Hein, K.R.G., and H. Spliethoff, "Co-combustion of Coal and Biomass in Pulverized Fuel and Fluidized Bed Systems," pp. 127-136 in *Combustion and Emissions Control II*, Proceedings of the Institute of Energy's *2nd International Conference*, Held in London UK, December 1995, Institute of Energy, London UK (1995).	FBC/Boilers Coal/Biomass Co-firing Performance
81730.	Gulyurtlu, I., C. Bardalo, E. Penha and I. Cabrita, "Co-combustion of Coals with Straw in a Fluidized Bed Combustor," pp. 137-147 in *Combustion and Emissions Control II*, Proceedings of the Institute of Energy's *2nd International Conference*, Held in London UK, December 1995, Institute of Energy, London UK (1995).	FBC Coal/Straw Co-firing Design Changes Performance Emissions

81731. Werther, J., T. Ogada, V.A. Borodulya and V.I. Dikalenko, "Devolatilization and Combustion Characteristics of Sewage Sludge in a Bubbling Fluidized Bed Furnace," pp. 149-158 in *Combustion and Emissions Control II*, Proceedings of the Institute of Energy's *2nd International Conference*, Held in London UK, December 1995, Institute of Energy, London UK (1995).

FBC
Sewage Sludge
Drying
Devolatilization
Combustion
Stages

81732. Zukowski, W., "Acoustic Effects During the Combustion of Gaseous Fuels in a Bubbling Fluidized Bed," *Combust. Flame* 117, 629-635 (1999).

FBC
Bubbling
C_3H_8 ,C_4H_{10} Fuels
Acoustic
Generation
Measurements

81733. Ilbas, M., P. Bowen, T. O'Doherty and N. Syred, "CFD Modeling of a Low NO_x Combustor Fired by Natural Gas and Gas-Oil," pp. 189-198 in *Combustion and Emissions Control II*, Proceedings of the Institute of Energy's *2nd International Conference*, Held in London UK, December 1995, Institute of Energy, London UK (1995).

Cyclone Combustor
Natural Gas
Gas/Oil Fuels
CFD Flowfields
NO_x Emissions
Model

81734. Twist, T.H., and K.J.A. Hargreaves, "Emissions Control and Its Implications on the Domestic Gas Burner Manufacturer," pp. 29-38 in *Combustion and Emissions Control II*, Proceedings of the Institute of Energy's *2nd International Conference*, Held in London UK, December 1995, Institute of Energy, London UK (1995).

Domestic
Appliance Burners
Low Emissions
New Designs

81735. Solero, G., and M. Beghi, "Experimental Fluid Dynamic Characterization of a Premixed Natural Gas Burner for Domestic and Semi-Industrial Applications," pp. 39-48 in *Combustion and Emissions Control II*, Proceedings of the Institute of Energy's *2nd International Conference*, Held in London UK, December 1995, Institute of Energy, London UK (1995).

Domestic Burner
Low NO_x
Lean CH_4/Air
Slotted Design
LDA Velocities

81736. Schadow, K., and W.R. Seeker, "Compact Waste Incinerator Technologies," pp. 239-251 in *ASME Proceedings of the 7th AIAA/ASME Joint Thermophysics and Heat Transfer Conference: Volume 1*, B.F. Armaly, S.C. Chan, D. Ezekoye, W. Gill, J. Gore, D.A. Kaminski, L. Phinney, S.T. Thynell, J.C. Yang and C.Q. Zhou, eds., 35 Papers Presented in Albuquerque NM, June 1998, ASME Publication HTD-Vol. 357-1, 305 pp., The American Society of Mechanical Engineers, New York NY (1998).

Incineration
Enhanced
Burning Rates
New Technologies

81737. Barham, P., J. David, K.J.A. Hargreaves, W.C. Maskell, R.N. Sauba and A. Suthenhiran, "Characterization of a 5 kW Gas Fired Pulsed Combustor: NO_x and CO Emissions," pp. 229-238 in *Combustion and Emissions Control II*, Proceedings of the Institute of Energy's *2nd International Conference*, Held in London UK, December 1995, Institute of Energy, London UK (1995).

Pulsed Combustor
Natural Gas
CO,NO_x
Emissions
A/F Dependence

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Pulsed Combustors
Natural Gas
CO,NO_x
Emissions

81739. In, V., M.L. Spano, J.D. Neff, W.L. Ditto, C.S. Daw, K.D. Edwards and K. Nguyen, "Maintenance of Chaos in a Computational Model of a Thermal Pulse Combustor," *Chaos* 7, 605-613 (1997).

Pulse Combustor
Flame Out
Control
Model

81740. Ahmed, S.A., and K.B. Abidogun, "Measurements of Turbulence Statistics and Energy Budgets in a Model Combustor," *Energy* 23, 741-752 (1998).

Dump Combustor
2-Component LDV
Turbulent
Kinetic Energy
Terms

81741. Fick, W., A.J. Beale, T. O'Doherty, A.J. Griffiths and N. Syred, "Studies of Resonant Coupling in Swirl Burner/Furnace Systems," pp. 229-238 in *Combustion and Emissions Control. III*, A Collection of 23 Papers, 350 pp., Institute of Energy, London UK (1997).

Swirl Burner
Precessing
Vortex Core/
Helmholtz
Instabilities
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Emissions

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N_2^+(B-X)
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Discharges

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(81768)	$Cu(s)/O_2$; Brass, Bronze/O_2	Ignition Temperatures
(81767)	Metals/F_2, Cu, Al, Ti, Mo, Ni, W/Nb, Fe, Steel	Ignition Temperatures
(81919)	Diesel Engine, Natural Gas Direct Injection, Diesel Fuel Pilot, NO_x Reductions	Pilot Ignition
(81784)	H_2/Air/Pt, Catalytic Combustion, Extinction, Modeling	Ignition
(81802)	$H_2/Cl_2/CH_2F_2/O_2$ Combustion, Hg Lamp Initiation, Flame Velocities	Photon Ignition

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Diffusion Flame
Fuel Side
Heat Loss
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12. TURBULENCE

(See also Section 14 for Turbulent Flowfields and Burning Velocities)

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(81735)	Domestic Burner, Low NO_x, Lean CH_4/Air, Slotted Design	LDA Velocities
(81740)	Turbulent Kinetic Energy Terms, Dump Combustor	2-Component LDV
(81805)	Jet Flames, Flow Structures, Axial Forcing, Flame Length	LDV
(81897)	I.C. Engine, Turbulent Length Scales, Measurements	LDV
(81898)	I.C. Engine, Velocities, Flowfield Measurements	LDV
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(See also Section 26 for Ion Spectroscopy, Section 27 for Penning Ionization, Section 40 for Dynamics of Ion-Molecule Reactions, Section 42 for MPI Processes, Section 43 for Ionic P.E. Curves, Section 44 for Ion Structures and Section 46 for Thermochemical Values)

(82265) $C_3H_4+h\nu$(193 nm), Product Ions and C_2(d-a), C_2(D-X), CH(A-X), C* Emission

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$(CD_3)_2CO,(S_2,S_1)$
State Lifetimes
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Fragment Probes
RRKM Analysis

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NH_3, ND_4
Photoionization
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O^-,O_2^-
Channels

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Inhibition
CF_3Br/Inert
CHF_3/Inert
Mixture Effects
Synergism

(82204) Inhibition, $CH_4/O_2/M$ Flames, Species Profiles, Emission, LIF, Kinetic Modeling
CF_4,CHF_3
CH_2F_2,CH_3F

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C_2H_4 Addition

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Additive Effects

(81969) FBC, NO Control Effects, Kinetics
Fe Particles

(81841) Detonation Cell Size, H_2/Air
H_2O_2,O_3
Additive Effects

(81970) NO_x Control Method, Na Enhancement Effects
NH_3/Na Additive

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NH_3/SO_2
Addition

17. CORROSION/EROSION/DEPOSITION

(See also Section 22 for Diamond Formation Deposition)

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Performance

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Modification
Performance
Recirculation
Overfire Air
Techniques

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Reburn Zone

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Effects

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Effects
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FBC
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Air Staging
Control Method

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Fluctuations
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Methodology

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Sizes,Shapes
Volume Fractions
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C_2H_4/Air
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Absorption
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Organosilicon
Precursor Effect
Surface Areas

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TiO_2
Particle Formation
CH_4/Air Flame
Nanosizes
Sintering Times

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Soot

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Method

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Temperatures
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Review

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Cement Blend
Disposal

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(See also Section 22 for Nucleation and Growth of Particles)

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BaKr,BaXe

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C_{44},C_{50}
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(82486)	Structural Calculations, Geometry, ΔH_f	$NO^+.N_2$
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(82419)	v,J Energy Levels, v≤25 Bound States, D_0, Calculations	$(O_2)_2$
(82420)	v,J Energy Levels, v=0,0 and 1,0 Dimers, Bound States, D_0	$(O_2(a))_2$
(82421)	Vibrational Energy Levels, Rg=Ar,Kr, Calculations	SH(A).Rg SD(A).Rg
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CaI(B,A-X)
Cross Sections
Branching Ratios
$Ca(^1P_1)+CH_3X$
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High Resolution
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C_6H_6 ,$C_6H_5CH_2$
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IR Emission
Dunham Constants
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CuOH
Rotational
Spectra
Geometries
Constants

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Absorption
Cross Sections
P.E. Curves
Calculations

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CF_3I
Rydberg States
$CF_3I^+(X)$
ZEKE-PFI
REMPI Spectra
Assignments
IP

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C_2F_6, $C_2H_2F_4$
C_2H_3F, $C_2H_3F_3$
$C_2H_4F_2$, C_3HF_7
$C_3H_6F_2$, C_3H_7F
$C_4H_5F_3$
Frequencies
Scaling Method

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2-Color RFWM
Spectrum
$N' \leq 23$ Analysis
Constants
Predissociation

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$CHCl_3$, ν_3
FTIR Spectrum
Band Center
Constants

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CHF(A-X)
LIF Spectrum
Beam Cooled
Frequencies

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CH_3SH, $(CH_3)_2S$
H_2, NH, N_2O, SH
PES/REMPI
Electronic Structure
Applications

(82339) Electronic Structure, Ultraviolet Spectrum, Calculations

CH_3SO_2

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CO
Dipole Moment
Calculations

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CO(A-X)
Emission Spectrum
Transition Moment
Probabilities

(82101) Rydberg States, Term Values, Predissociation, Calculations

$CO(C^1\Sigma^+, B^1\Sigma^+)$

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CO_2,7580 cm^{-1}
H_2O,7529 cm^{-1}
Cavity Enhanced
Absorption
Spectra

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C_2H_2
Intracavity
Absorption
Vibrational
Level Assignments
Constants

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C_2H_2(A-X)
LIF,REMPI
Spectra
cis-,trans CH
Bending
Progressions

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C_2H_2
Electronic States
Low-lying
Singlets/Triplets
Geometries
Calculations

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c-$C_2H_2N_4$
47 Excited
Electronic States
Energies
Calculations

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CF_3CH_3
IR,Raman
Spectra
Frequencies
Assignments

(82227) Infrared Spectra, Measurements

$CF_3OCH_2O_2NO_2$
$CF_3OC(O)O_2NO_2$

(82531) Photoelectron Spectrum, Analysis, IP

C_2H_3Cl

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$C_2H_4Cl_2$
FT Absorption
Frequency
Assignments

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CH_3CHO
Rotational
Quantum Numbers
Labeling Method

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C_2H_4O
VUV Photoionization
Spectrum
Product Ions
APS

(82229) Ultraviolet Absorption Cross Section

CH_2CCH

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$CF_3C(O)OCHCF_3$
$CF_3C(O)OCHO_2CF_3$
UV Absorption
Cross Sections
$CF_3C(O)OCH_2CF_3 + F$
$2\ CF_3C(O)OCHCF_3$
$2\ CF_3C(O)OCHO_2CF_3$
$CF_3C(O)OCH_2O_2CF_3 + M$
$M = NO, NO_2$
Rate Constants

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c-C_6H_7
UV Absorption
Cross Sections
$C_6H_7 + C_6H_7$
Rate Constant
$C_6H_7 / C_6H_6 + H$
Equilibrium
$\Delta H_f(c\text{-}C_6H_7)$

(82232) Ultraviolet Absorption Cross Sections

$C_6H_5C(O)O_2$

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$C_{10}H_8^+$
Absorption
Spectrum
Cavity Ringdown

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$CaCH_3(X)$
Rotational
Spectrum
Constants

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ClO(A-X)
Absorption
Cavity Ringdown
Spectral Constants
Lifetimes
Predissociation

82044. Muller, H.S.P., E.A. Cohen and D. Christen, "The Rotational Spectrum of Chloryl Chloride, $ClClO_2$, in its Ground Vibrational State," *J. Chem. Phys.* 110, 11865-11875 (1999).

$ClClO_2(X,v=0)$
Rotational Spectrum
Constants
Isotopes

(81860) Photodetachment Spectrum, $Cl_3(1^2\Sigma,X)$ States

Cl_3^-

82045. Sousa, C., W.A. De Jong, R. Broer and W.C. Nieuwpoort, "Charge Transfer and Relativistic Effects in the Low-lying Electronic States of CuCl, CuBr and CuI," *Mol. Phys.* 92, 677-686 (1997).

CuCl,CuBr
CuI
Electronic Transitions
Low-lying States
Energies
Calculations

82046. Zhou, M., and L. Andrews, "Reactions of Laser Ablated Iron Atoms and Cations with Carbon Monoxide: Infrared Spectra of $FeCO^+$, $Fe(CO)_2^+$, $Fe(CO)_x$ and $Fe(CO)_x^-$ (x=1-4) in Solid Neon," *J. Chem. Phys.* 110, 10370-10379 (1999).

$FeCO,FeCO^{\pm}$
$Fe(CO)_2,Fe(CO)_2^{\pm}$
FTIR Spectra
Frequencies
Matrix Study

82047. Mochizuki, Y., and K. Tanaka, "Theoretical Investigation on the GaH Molecule and Its Positive Ion," *Theor. Chem. Acc.* 99, 88-94 (1998).

GaH,GaH^+
Spectral Constants
IP,D_e
Calculations

82048. Hupper, B., and B. Eckhardt, "Uniform Semiclassical Calculation of the Direct Part of the Photodissociation Cross Section of Water," *J. Chem. Phys.* 110, 11749-11755 (1999).

$H_2O(A-X)$
Photodissociation
Cross Sections
Calculations

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$He(2^3P_{1,0})$
Energy Splitting
Microwave Spectrum

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IBr
FTIR Spectrum
$v'=1-3$ Bands
Analysis

82051. Newman, S.M., W.H. Howie, I.C. Lane, M.R. Upson and A.J. Orr-Ewing, "Predissociation of the $A^2\Pi_{3/2}$ State of IO Studied by Cavity Ringdown Spectroscopy," *J. Chem. Soc., Faraday Trans.* 94, 2681-2688 (1998).

IO(A-X)
Cavity Ringdown Absorption
$v'=0-5,v''=0,1$
Spectral Constants
Predissociation
Lifetimes
Mechanism

(82244) 445 nm Absorption Cross Section Measurement

IO

82052. Citra, A., and L. Andrews, "Reactions of Laser Ablated Iridium Atoms with O_2: Infrared Spectra and DFT Calculations for Iridium Dioxide and Peroxo Iridium (VI) Dioxide in Solid Argon," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 4182-4190 (1999).
IrO_2, IrO_4
FTIR Spectra
Frequency Assignments
Matrix Study

82053. Wang, X., H. Wang, P.L. Gould, W.C. Stwalley, E. Tiesinga and P.S. Julienne, "Observation of the Pure Long-Range 1_u State of an Alkali Metal Dimer by Photoassociative Spectroscopy," *Phys. Rev. A: At. Mol. Opt. Phys.* 57, 4600-4603 (1998).
$K_2(1_u)$
Photoassociative RE2PI Spectrum
Constants
D_e

82054. Reddic, J.E., and M.A. Duncan, "Photodissociation Spectroscopy of the Mg^+-Ne Complex," *J. Chem. Phys.* 110, 9948-9955 (1999).
Mg^+Ne(B,A-X)
Photodissociation Spectra
D_0(A,X)
Constants

82055. Andrews, L,. and M. Zhou, "Reactions of Laser Ablated Molybdenum and Tungsten Atoms with Nitric Oxide: Infrared Spectra of the MN, NMO and M-η^1-$(NO)_x$ (x=1,2,3,4) Molecules and $(NO)_2^+$ and $(NO)_2^-$ Ions in Solid Argon," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 4167-4173 (1999).
MoN,OMoN
WN,OWN
FTIR Spectra
Frequencies
Matrix Study

82056. Andrews, L., P.F. Souter, W.D. Bare and B. Liang, "Reactions of Laser-Ablated Mo and W Atoms with Dinitrogen: Infrared Spectra of Metal Nitrides, Dinitrides and Complexes in Solid Argon and Nitrogen," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 4649-4658 (1999).
MoN,WN
MoN_2, WN_2
FTIR Spectra
Frequencies
Matrix Study

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MoO^+
3 Lowest-Lying Electronic States
Spectral Constants
IP(MoO)
Calculations

82058. Plemmons, D.H., C. Parigger, J.W.L. Lewis and J.O. Hornkohl, "Analysis of Combined Spectra of NH and N_2," *Appl. Opt.* 37, 2493-2498 (1998).
NH(A-X)
N_2(C-B)
Deconvolution
Overlapping Spectra
Method

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NH_3, $\nu_1+\nu_3$
NH_3, $\nu_1+2\nu_4$
Cavity Enhanced Absorption Spectra

82060.	Takazawa, K., and H. Abe, "Electronic Spectra of Gaseous Nitric Oxide in Magnetic Fields up to 10 T," *J. Chem. Phys.* 110, 9492-9499 (1999).	NO(A-X),(0,0) LIF Spectrum Zeeman Effects Assignments
82061.	Danielak, J., R. Kepa and M. Zachwieja, "New Spectroscopic Studies of the γ-Band System ($A^2\Sigma^+$-$X^2\Pi$) of the $^{15}N^{16}O$ Molecule," *J. Phys. B. At. Mol. Opt. Phys.* 30, 4889-4898 (1997).	^{15}NO(A-X) Emission Spectrum Constants F.C. Factors *r*-Centroids Measurements
82062.	Hippler, M., and J. Pfab, "Electronic Spectroscopy of the C-State of NO by Laser Multiphoton Ionization: Rotational Structure of the $C^2\Pi$ ($v'=0$)$\leftarrow X^2\Pi$($v''=0$) Two-Photon Band," *Mol. Phys.* 94, 313-323 (1998).	NO(C-X) (2+1) REMPI Spectrum Jet Cooled Constants
82063.	Mojarrabi, B., L. Campbell, P.J.O. Teubner, M.J. Brunger and D.C. Cartwright, "Erratum-Differential and Integral Cross Sections for Excitation of the Electronic States of Nitric Oxide by Low-Energy Electron Impact: Observation of a ($^2\Pi_r \rightarrow {}^2\Phi$) Excitation Process [*Phys. Rev. A: At. Mol. Opt. Phys.* 54, 2977-2982 (1996)]," *ibid.* A58, 1609 (1998).	NO($L'\ {}^2\Phi$) Observations Erratum
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82067.	Chupka, W.A., and E.R. Grant, "Anomalous Intensities in Zero-Kinetic-Energy Spectra," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 6127-6133 (1999).	NO_2 ZEKE Spectrum Anomalous Intensities Explanations
82068.	Fulara, J., L. Lapinski, O. Morawski and J. Prochorow, "Cavity Ringdown Measurement of the ($B^2\Sigma_u{}^+$-$X^2\Sigma_g{}^+$),(1,0) Absorption Band of the $N_2{}^+$ Cation," *Acta Phys. Pol. A* 93, 723-730 (1998).	$N_2{}^+$(B-X),(1,0) $N_2{}^+$(A-X),(4,0) Cavity Ringdown Spectra

82069.	Tamanis, M., M. Auzinsh, I. Klincare, O. Nikolayeva, R. Ferber, E.A. Pazyuk, A.V. Stolyarov and A. Zaitsevskii, "NaK Λ-Doubling and Permanent Electric Dipoles in Low-lying $^1\Pi$ States: Experimental and Theory," *Phys. Rev. A: At. Mol. Opt. Phys.* 58, 1932-1943 (1998).	$NaK(D^1\Pi,v)$ RF ODR/LIF Spectra Dipole Moments Measurements
82070.	Pashov, A., I. Jackowska, W. Jastrzebski and P. Kowalczyk, "Polarization Labeling Spectroscopy of the $3^1\Pi$ and $6^1\Sigma^+$ States in NaK," *Phys. Rev. A: At. Mol. Opt. Phys.* 58, 1048-1054 (1998).	$NaK(6^1\Sigma^+\text{-}X^1\Sigma^+)$ $NaK(3^1\Pi\text{-}X^1\Sigma^+)$ Absorption Polarization Labeled Spectra Constants P.E. Curves
82071.	Xing, D., Q. Wang, S. Tan and K.-i. Ueda, "Triplet-State Bound-Free Transitions of Alkali Dimers (Na_2, K_2 and Rb_2) by Electron Beam Excitation," IEEE *J. Quantum Electron.* 34, 1765-1771 (1998).	$Na_2(2^3\Pi_g\text{-}a^3\Sigma_u^+)$ K_2,Rb_2 Assignments Alkali/Ar/e^- Excitation
82072.	von Busch, H., V. Dev, H.-A. Eckel, S. Kasahara, J. Wang, W. Demtroder, P. Sebald and W. Meyer, "Unambiguous Proof for Berry's Phase in the Sodium Trimer: Analysis of the Transition ($A^2E''\leftarrow X^2E'$)," *Phys. Rev. Lett.* 81, 4584-4587 (1998); 82, 3560 (1999).	Na_3(A-X) v,J Structure Calculations Data Comparison
(82200)	415-545 nm Optogalvanic Spectrum, Assignments	Ne
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(82542)	Spectral Constants, Geometries, Energies, EAs, Calculations	PN,PN^- SiO,SiO^-
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82076. Klopcic, S.A., V.D. Moravec and C.C. Jarrold, "Photoelectron Spectrum of PdO^-," *J. Chem. Phys.* 110, 10216-10217 (1999).

PdO^-
Photoelectron Spectrum
Assignments
Energies

82077. Sjovoll, M., H. Fagerli, O. Gropen, J. Almlof, J. Olsen and T.U. Helgaker, "Spin-Orbit and Correlation Effects in Platinum Hydride, PtH," *Int. J. Quantum Chem.* 68, 53-64 (1998).

PtH
Low-lying Electronic States
Spin-Orbit Splitting
Energies, r_e
Calculations

82078. Bare, W.D., A. Citra, G.V. Chertihin and L. Andrews, "Reactions of Laser-Ablated Platinum and Palladium Atoms with Dioxygen: Matrix Infrared Spectra and Density Functional Calculations of Platinum Oxides and Complexes and Palladium Complexes," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 5456-5462 (1999).

PtO, PtO_2
PtO_3
FTIR Spectra
Frequencies
Matrix Study

82079. Citra, A., and L. Andrews, "Reactions of Laser Ablated Rhodium Atoms with O_2: Infrared Spectra and DFT Calculations for RhO, ORhO, $(O_2)RhO_2$, Rh_2O_2, $Rh(O_2)$ and $(O_2)Rh(O_2)$ in Solid Argon," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 4845-4854 (1999).

RhO, RhO_2
RhO_4, Rh_2O_2
FTIR Spectra
Frequencies
Matrix Study

82080. Li, Q., Q. Zhang, J. Shu, S. Yu, Q. Song, C. Chen and X. Ma, "A New Excited Electronic State of SF_2 Radical Observed by Resonance Enhanced Multiphoton Ionization," *Chem. Phys. Lett.* 305, 79-84 (1999).

SF_2(B′-X)
REMPI Spectrum
Band Origin
Frequencies
Predissociation

82081. Khriachtchev, L., M. Pettersson, E. Isoniemi, J. Lundell and M. Rasanen, "Laser Induced Fluorescence Studies of S_2^+ in Solid Argon," *Chem. Phys. Lett.* 302, 324-330 (1999).

S_2^+(A-X)
LIF Spectrum
Lifetime
Matrix Study

82082. Bauschlicher Jr, C.W., M. Zhou, L. Andrews, J.R.T. Johnson, I. Panas, A. Snis and B.O. Roos, "A Further Study of the Products of Scandium and Dioxygen Reactions," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 5463-5467 (1999).

ScO^+, ScO_2^+
ScO_2^-, ScO_3
FTIR Spectra
Frequencies
Matrix Study

82083. Palmieri, P., R. Tarroni, A.O. Mitrushenkov and T. Thorsteinsson, "A Multireference Configuration Interaction Study of the Fine Structure of the ($A^2\Pi_u \leftarrow X^2\Sigma_g^+$) Transition of the Si_2^- Anion," *J. Chem. Soc., Faraday Trans.* 94, 3061-3066 (1998).

Si_2^-(A-X)
(2,0),(1,0)
Fine Structure
Calculations

82084. Dupuis, M., and J.B. Nicholas, "On the Electronic Structure of Si_3O_2 and Its Anion," *Mol. Phys.* 96, 549-553 (1999).

Si_3O_2
$Si_3O_2^-$
Electronic States
Assignments
Photoelectron
Detachment
Spectrum
Calculations

82085. Beardah, M.S., and A.M. Ellis, "Observation of Several New Electronic Transitions of the SrOH Free Radical," *J. Chem. Phys.* 110, 11244-11254 (1999).

SrOH(F,E,D,C-X)
LIF Spectra
Assignments
Constants

82086. Han, Y.-K., C. Bae and Y.S. Lee, "On the Consistent Definition of Spin-Orbit Effects Calculated by Relativistic Effective Core Potentials with One-Electron Spin-Orbit Operators: Comparison of Spin-Orbit Effects for Tl, TlH, TlH_3, PbH_2 and PbH_4," *J. Chem. Phys.* 110, 9353-9359 (1999).

Tl,TlH,TlH_3
PbH_2,PbH_4
Spin-Orbit Splitting
Calculations

82087. Davico, G.E., R.L. Schwartz, T.M. Ramond and W.C. Lineberger, "An Experimental Study of the Low-lying Electronic States of WO_2," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 6167-6172 (1999).

WO_2
4 Low-lying
Electronic States
WO_2^- PES
Spectra
State Geometries
Frequencies
Assignments

82088. Jonin, C., P. Laporte and F. Spiegelmann, "Transient Visible Spectroscopy from $(1)0_u^-$, $(1)1_u$ and $(1)0_u^+$ States of Xe_2* in the Range 500-600 nm," *Chem. Phys. Lett.* 308, 13-20 (1999).

Xe_2
LIF Spectra
State
Assignments

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$ZnNe(^1\Sigma^+)$
$ZnNe(^1\Pi)$
LIF Spectra
Constants
Bond Lengths
D_0

82090. Kushto, G.P., and L. Andrews, "Infrared Spectroscopic and Density Functional Theoretical Investigation of the Reaction Products of Laser Ablated Zr, Hf and Th Atoms with Nitric Oxide," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 4836-4844 (1999).

NZrO,NHfO
NThO
FTIR Spectra
Frequencies
Matrix Study
Zr,Hf,Th + NO

82091. Beaton, S.A., and M.C.L. Gerry, "Rotational Spectra and Hyperfine Constants of ZrO and ZrS," *J. Chem. Phys.* 110, 10715-10724 (1999).

ZrO,ZrS
Rotational
Spectrum
Isotopomers
Constants

(See also Section 45 for Vibrational and Rotational Relaxation Processes)

(82316)	Reaction Dynamics, Steric Effects, CF_3* Product Channel	$Ar(^3P)+CHF_3$
82092.	Zhang, Y., Y. Yoon, P.B. Kelly and I.M. Kennedy, "Measurement of Quenching Cross Sections for Laser Induced Fluorescence of Atomic Arsenic," *Appl. Opt.* 37, 7132-7136 (1998).	$As(^4P_{1/2})+M$ Quenching Cross Sections $M=CH_4, CO, C_2H_4, H_2, N_2$
82093.	Niday, T.A., and D.E. Weeks, "Scattering Matrix Elements for the Fine Structure Transition $B(^2P_{1/2})+H_2(j=0)\leftrightarrow B(^2P_{3/2})+H_2(j=0)$," *Chem. Phys. Lett.* 308, 106-114 (1999).	$B(^2P_{1/2})+H_2$ (1/2,3/2) Mixing Probabilities Calculations
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(82427)	9 Low-lying States, Lifetimes, P.E. Curves, Spectral Constants, Calculations	BiS
(82319)	Reaction Dynamics, Probabilities, Four Models Tested, Accuracies	$Br(^2P_{1/2})+H_2$
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(82320)	Reaction Dynamics, P.E. Surfaces, Channels, Energies	$C(^1D)+H_2O$ $C+H_2O$
(82428)	Lifetimes, Predissociations, P.E. Curves, Calculations	$CF(2^2\Sigma^+,D,B,A)$
(82024)	Predissociation, 2-Color RFWM Spectrum, $N'\leq 23$, Analysis, Constants	CH(C,v=1)
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(82546)	LIF Electric Field Quenching, Orientation	*c*-$C_4H_4N_2$
(82432)	Lifetime, P.E. Surfaces, Low-lying States, $^1A_1$ / $^3B_1$ Crossing Point	$C_6H_5^+(^3B_1)$
(82010)	Cross Sections, Product Branching Ratios, CaCl, CaI(B,A-X) Chemiluminescence, Reactant Alignment Effects	$Ca(^1P_1)+CH_3X$
(82496)	E-E Pooling, $(^1P_1)$ Product Cross Sections, Polarization Effects	$Ca(^3P_1)+Ca(^3P_1)$
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(82355)	Reaction Dynamics, P.E. Surfaces, Energy Barriers	$Cd(^{1,3}P,^1S_0)+SiH_4$ $Hg(^{1,3}P,^1S_0)+SiH_4$
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(82043)	Predissociation Lifetimes, Cavity Ringdown Absorption, (A-X) Spectral Constants	ClO(A)
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Relaxation
Rate Constants
Calculations

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Product OH(X,v,N,f)
Distributions
Polarizations
Measurements
Calculations

(82357) Rate Constants, Reaction Dynamics, Theoretical Methods, Accuracies
$O(^1D)+H_2$

(82518) Rotational Energy Transfer, ps LIF, CH_4/O_2, Air Flame, Rate Constants, Energy Gap Law
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Channels
Cross Sections
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Measurements

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(82385)	Reaction Dynamics, Transition States, Stabilities, Mechanism	$^1O_2+C_2H_4$
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(82497)	E-E Transfer, $Rb(5^2D)$ Product Cross Sections, Calculations	$Rb(7^2S)+Rb$

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(82080) Predissociation, REMPI Spectrum, (B′-X) Band Origin, Frequencies — SF_2(B′)

(82454) Predissociation, P.E. Surfaces, Stationary Points, Double Minimum Potential — SO_2(C)

(82081) Lifetime, LIF Spectrum, Matrix Study — S_2^+(A)

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28. FRANCK-CONDON FACTORS/TRANSITION PROBABILITIES

(See also Section 27 for Lifetimes and Transition Probabilities)

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Oscillator Strengths
$v'=11\text{-}23, v''=0$
Measurements

(82029) Transition Moment Probabilities, Emission Spectrum
CO(A-X)

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Band Oscillator Strengths
Broadening Coefficients
Measurements

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C_2H^-

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Co^+
Forbidden Radiative Transition Probabilities
Calculations

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Absorption
Transition Strength Ratio
Measurement

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IF(B-X)
ICl(B-X)
Transition Moments
Calculations

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I_2
fs Pump/Probe

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Oscillator Strengths
Calculations
Data Comparisons

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Spectral Transitions
Oscillator Strengths
Calculations

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O($4p^3P$-$3s^3S$)
Transition
Probabilities
Measurements

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Absorption
Oscillator
Strengths
Cross Sections

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O_2(B,A′,A,$1^3\Pi_u$-b)
Transition
Dipole Moments
Calculations

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O_2(a-X),liquid
Collision Induced
Enhancements
Mechanism

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S
Oscillator
Strengths
Calculations

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SiF(D-X)
SiN(D-A)
F.C. Factors
r-Centroids
Calculations

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Ti
92 Transition
Probabilities
Measurements

29. LINESHAPES/STRENGTHS

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(82177) Broadening Coefficients, Absorption, Diode Lasers, Monitoring — CO_2, H_2O

(82231) FTIR Band Intensities, Ethylene Glycol Diformate — $(HCOOCH_2)_2$

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(82178)	Lineshape Models, Absorption, Diode Laser, High Pressure Flame Gases, Monitor	H_2O
(82110)	Rotational Predissociation Linewidths, OH(A) Product Branching Ratios	H_2O(C-X)
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(82074)	Line Strengths, Cavity Ringdown Absorption Spectrum, Detection Limits	O_2(b-X),(2,1,0-0)

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REMPI
Hg
New Method
Monitoring
Assessment

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FTIR
CH_4,CO,H_2O
CO_2,NO
Flare Emission
Monitor

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FTIR
Diode Lasers
DOAS Absorption
Atmospheric
Monitoring
Methods

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Absorption
Intracavity
Laser Spectroscopy
Techniques
Monitoring
Reviews

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Absorption
Cavity Ringdown
CH(C-X)
CH_4/Air Flame
Sensitivity

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CH
Cavity Ringdown

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Absorption
CH_4,CO,CO_2
Diode Laser
Overtone/
Combination Bands
CH_4/Air Flames

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Absorption
CO
Diode Laser
Monitor

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Absorption
CO,HC,NO_2
Diode Laser
Roadside
Auto Monitor

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Absorption
CO, CO_2
Diode Lasers
Frequency
Modulation
Multiplexing

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Absorption
CO_2, H_2O
Diode Lasers
Broadening
Coefficients
Monitoring

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Absorption
H_2O
Diode Laser
High Pressure
Flame Gases
Lineshape Models
Monitoring

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Absorption
NO(3,0)
Diode Laser
Sensitivity

(82074) Cavity Ringdown, (2,1,0-0) Bands, Line Strengths, Detection Limits

Absorption
O_2(b-X)

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Absorption
Rb($^2P_{3/2}$-$^2S_{1/2}$)
Diode Laser
T,Velocities
Hypersonic Flows

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Absorption
SiH_2
Laser Intracavity
Cavity Ringdown
SiH_4/Ar Discharge
Monitoring Methods
Comparisons
Dust Particles

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Fragmentation
LIF
193 nm Laser
Au,Pb
H_2SO_4 Aerosol
Monitor

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LIF
Plasma Diagnostic
Brief Guide
CF, CF_2, N_2^+

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2-Photon LIF
CO
C_3H_8/Air
CO_2 Photolytic Interference

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LIF
H_α
Arcjet Nozzle
Velocities
e^- Densities

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Fragmentation
LIF
NH_3
NH(A-X) Emission
Quenching Factors
Sensitivity

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LIF
NO
CH_4/Air
CH_3Cl, CH_2Cl_2
Photochemical Interferences

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PLIF
Linear/
Saturated
NO
Spray Flame
Comparisons

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LIF
Linear/Saturated
NO
Comparisons
C_2H_6/Air Flame

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2-Photon LIF
NO
Monitoring
Method

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LIF
$N_2(A,v=4)$
Monitor
(B-A) Transition
RF Discharge

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Raman
Rich CH_4/Air
Sooting Flame
Major Species
Temperatures

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SRS
O_2(a,X)
Monitor
O_2(a)/I Laser

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CARS
CH_4, N_2
Simultaneous
Monitor

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Polarization
Sensitive CARS
NO
Monitor
N_2 Discharge/NO
Interactions

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CARS
Rotational
Na Seeded Flame
Stray Light Filter

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DFWM
OH(A-X),(0,0)
Polarization
Spectral
Measurements
CH_4/Air
H_2/O_2 Flames

31. FLAME CONCENTRATION MEASUREMENTS

(See also Section 34 for Flame Species Profiles)

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CH
Concentrations
CH_4 Diffusion
Flame
Cavity Ringdown
Absorption

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Species Profiles
C_6H_6/Air
Rich Flames
PAHS,Soot
Probe Sampling

32. MAPPING/TOMOGRAPHIC METHODS

33. OPTOGALVANIC/OPTOACOUSTIC METHODS

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Optogalvanic
Spectrum
Ne
415-545 nm
Assignments

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Kinetic Modeling
CH_4/Air
Mechanism
Reduction
Algorithm

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Kinetic Modeling
CH_4/Air
NO Formation

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Kinetic Modeling
CH_4/Air
NO_x Formation
Reduced Schemes
Thermal,Prompt
Fuel N,Reburn
Roles

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Kinetic Modeling
CH_4/O_2/RF
RF=CH_3F,CH_2F_2,
CHF_3,CF_4
Inhibition
Species Profiles
Emission,LIF

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35. PYROLYSIS KINETICS/STUDIES

(81757) Kinetic Parameters, Rates — Biomass Pyrolysis

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(82206) Pyrolysis, Shock Tube, Species Profiles, Kinetic Modeling — C_2H_4; C_2H_4/O_2

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(81996) Pyrolysis, Soot Aggregation Mechanisms — C_6H_6/N_2

36. KINETIC MODELING/SENSITIVITIES/RATE CONSTANTS

(See also Section 15 for Ion Reaction Rate Constants, Section 27 for Excited State Rate Constants, Section 39 for Unimolecular Rate Constants, Section 40 for Theoretically Calculated Values and Section 45 for Energy Relaxation Rate Constants)

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CH_3+O
Rate Constant
HCHO,CO
Reaction Products

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CH_3+O_2
Rate Constants
T Dependence
Shock Tube

82222. Michael, J.V., S.S. Kumaran and M.-C. Su, "Rate Constants for $CH_3+O_2 \rightarrow CH_3O+O$ at High Temperature and Evidence for $H_2CO+O_2 \rightarrow HCO+HO_2$," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 5942-5948 (1999).
CH_3+O_2
Rate Constants
T Dependence
Channels
$HCHO+O_2$
Reaction Evidence

82223. Caralp, F., M.-T. Rayez, W. Forst, N. Gomez, B. Delcroix, C. Fittschen and P. Devolder, "Kinetic and Mechanistic Study of the Pressure and Temperature Dependence of the Reaction CH_3O+NO," *J. Chem. Soc., Faraday Trans.* 94, 3321-3330 (1998).
$CH_3O+NO+M$
CH_3O+NO
Two Channel
Rate Constants
P,T Dependence
RRKM Analysis

82224. Scholtens, K.W., B.M. Messer, C.D. Cappa and M.J. Elrod, "Kinetics of the CH_3O_2+NO Reaction: Temperature Dependence of the Overall Rate Constant and an Improved Upper Limit for the CH_3ONO_2 Branching Channel," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 4378-4384 (1999).
CH_3O_2+NO
Rate Constant
T Dependence
$\leq$3% CH_3ONO_2
Product

82225. Martinez, E., J. Albaladejo, E. Jimenez, A. Notario and A. Aranda, "Kinetics of the Reaction of CH_3S with NO_2 as a Function of Temperature," *Chem. Phys. Lett.* 308, 37-44 (1999).
CH_3S+NO_2
Rate Constants
T Dependence
P Independence

82226. Crowley, J.N., G. Saueressig, P. Bergamaschi, H. Fischer and G.W. Harris, "Carbon Kinetic Isotope Effect in the Reaction CH_4+Cl: A Relative Rate Study Using FTIR Spectroscopy," *Chem. Phys. Lett.* 303, 268-274 (1999).
CH_4+Cl
$^{13}CH_4+Cl$
Kinetic Isotope
Effect Ratio
Measurement

82227. Christensen, L.K., T.J. Wallington, A. Guschin and M.D. Hurley, "Atmospheric Degradation Mechanism of CF_3OCH_3," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 4202-4208 (1999).
CF_3OCH_3+Cl
$CF_3OC(O)H+Cl$
$CF_3OC(O)O_2NO_2 \rightarrow$
$CF_3OC(O)O_2+HO_2$
Rate Constants
$CF_3OCH_2O_2NO_2$
$CF_3OC(O)O_2NO_2$
IR Spectra

82228.	Hynes, R.G., J.C. Mackie and A.R. Masri, "Shock Tube Study of the Oxidation of C_3F_6 by N_2O," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 5967-5977 (1999).	C_3F_6+O Rate Constants Branching Ratio Products Kinetic Modeling Shock Tube
82229.	Atkinson, D.B., and J.W. Hudgens, "Rate Coefficients for the Propargyl Radical Self-Reaction and Oxygen Addition Reaction Measured Using Ultraviolet Cavity Ringdown Spectroscopy," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 4242-4252 (1999).	$C_3H_3+C_3H_3$ C_3H_3+Br $C_3H_3+C_3H_3Br_2$ $C_3H_3+C_3H_3Cl_2$ $C_3H_3+O_2$,H Rate Constants C_3H_3 UV Absorption Cross Section
(82211)	Rate Constants, Pyrolysis Measurements, RRKM Analysis, Kinetic Model	CH_3CCH
82230.	Sauer, C.G., I. Barnes, K.H. Becker, H. Geiger, T.J. Wallington, L.K. Christensen, J. Platz and O.J. Nielsen, "Atmospheric Chemistry of 1,3-Dioxolane: Kinetic, Mechanistic and Modeling Study of OH Radical Initiated Oxidation," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 5959-5966 (1999).	*c*-$C_3H_6O_2+OH$,Cl $C_2H_4CO_3+Cl$ $CH_2(OCHO)_2+Cl$ Rate Constants Product Yields
(82039)	Rate Constants, M = NO, NO_2	$CF_3C(O)OCH_2CF_3+F$ 2 $CF_3C(O)OCHCF_3$ 2 $CF_3C(O)OCHO_2CF_3$ $CF_3C(O)OCH_2O_2CF_3+M$
82231.	Maurer, T., H. Hass, I. Barnes and K.H. Becker, "Kinetic and Product Study of the Atmospheric Photooxidation of 1,4-Dioxane and Its Main Reaction Product Ethylene Glycol Diformate," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 5032-5039 (1999).	*c*-$C_4H_8O_2+OH$ $(HCOOCH_2–)_2+OH$,Cl Rate Constants Products,Yields FTIR Band Intensities
(82040)	Rate Constant	$C_6H_7+C_6H_7$
82232.	Caralp, F., V. Foucher, R. Lesclaux, T.J. Wallington and M.D. Hurley, "Atmospheric Chemistry of Benzaldehyde: Ultraviolet Absorption Spectrum and Reaction Kinetics and Mechanisms of the $C_6H_5C(O)O_2$ Radical," *Phys. Chem. Chem. Phys.* 1, 3509-3517 (1999).	$C_6H_5CO+Cl_2$ 2 $C_6H_5C(O)O_2$ $C_6H_5C(O)O_2+NO,NO_2$ $C_6H_5C(O)Cl+Cl$ $C_6H_5C(O)O_2NO_2\rightarrow$ Rate Constants $C_6H_5C(O)O_2$ UV Absorption Cross Sections

82233. Vinckier, C., J. Helaers and J. Remeysen, "Kinetic Study of $Ca(^1S)+N_2O$ and $Sr(^1S)+N_2O$ Reactions in the Temperature Ranges of, Respectively, 303-1015 and 303-999 K," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 5328-5335 (1999).

$Ca+N_2O$
$Sr+N_2O$
Rate Constants
T Dependences
Two Channel Contributions

82234. Taatjes, C.A., "Infrared Frequency-Modulation Measurements of Absolute Rate Coefficients for $Cl+HD \rightarrow HCl(DCl)+D(H)$ between 295 and 700 K," *Chem. Phys. Lett.* 306, 33-40 (1999).

$Cl+HD$
Rate Constants
Product HCl/DCl Branching Ratio

82235. Kegley-Owen, C.S., M.K. Gilles, J.B. Burkholder and A.R. Ravishankara, "Rate Coefficient Measurements for the Reaction $OH+ClO \rightarrow$Products," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 5040-5048 (1999).

$ClO+OH$
Rate Constants
T Dependence

82236. Nesbitt, F.L., R.P. Thorn Jr, W.A. Payne Jr and D.C. Tardy, "Absolute Rate Constant and Product Branching Fractions for the Reaction between F and C_2H_4 at 202-298 K," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 4470-4479 (1999).

$F+C_2H_4$
Rate Constants
T Dependence
Branching Ratios

82237. Persky, A., "Erratum - Kinetics of the Reactions $F+H_2S$ and $F+D_2S$ at 298 K [*Chem. Phys. Lett.* 298, 390-394 (1998)]," *ibid.* 306, 416 (1999).

$F+H_2S$
$F+D_2S$
Rate Constants
Erratum

82238. Badenes, M.P., E. Castellano, C.J. Cobos, A.E. Croce and M.E. Tucceri, "Rate Coefficient for the Reaction $FCO+FC(O)O_2 \rightarrow 2FC(O)O$ at 296 K," *Chem. Phys. Lett.* 303, 482-488 (1999).

$FCO+FC(O)O_2$
$FC(O)O+FC(O)O_2+M$
Rate Constants
$\Delta H_f(FC(O)O_2)$
$\Delta H_f((FCO)_2O_2)$

82239. Arthur, N.L., and L.A. Miles, "Arrhenius Parameters for $H+(CH_3)_3GeH$ and $(CH_3)_2GeH_2$," *J. Chem. Soc., Faraday Trans.* 94, 2741-2744 (1998).

$Ge(CH_3)_3H+H$
$Ge(CH_3)_2H_2+H$
Rate Constants
T Dependences
Measurements

82240. Wrede, E., L. Schnieder, K.H. Welge, F.J. Aoiz, L. Banares, J.F. Castillo, B. Martinez-Haya and V.J. Herrero, "The Dynamics of the Hydrogen Exchange Reaction at 2.20 eV Collision Energy: Comparison of Experimental and Theoretical Differential Cross Sections," *J. Chem. Phys.* 110, 9971-9981 (1999).

'Hot' $H+D_2$
Crossed Beam
D Product Energies
Cross Sections

82241. Inomata, S., and N. Washida, "Rate Constants for the Reactions of NH_2 and HNO with Atomic Oxygen at Temperatures between 242 and 473 K," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 5023-5031 (1999).

$HNO+O$
NH_2+O
Rate Constants
Measurements

82242. Peng, J., X. Hu and P. Marshall, "Experimental and ab Initio Investigations of the Kinetics of the Reaction of H Atoms with H_2S," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 5307-5311 (1999).

H_2S+H
Rate Constants
T Dependence
Transition State

82243. Sommar, J., M. Hallquist, E. Ljungstrom and O. Lindqvist, "On the Gas Phase Reactions between Volatile Biogenic Mercury Species and the Nitrate Radical," *J. Atm. Chem.* 27, 233-247 (1997).

$Hg+NO_3$
$Hg(CH_3)_2+NO_3$
Rate Constants
Products
Atmospheric
Roles

82244. Atkinson, D.B., J.W. Hudgens and A.J. Orr-Ewing, "Kinetic Studies of the Reactions of IO Radicals Determined by Cavity Ringdown Spectroscopy," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 6173-6180 (1999).

IO+IO
IO+NO
CF_3I+O
Rate Constants
IO Absorption
Cross Section

82245. Balakrishnan, N., and A. Dalgarno, "Rate Coefficients for NO Formation in Energetic $N+O_2$ Collisions," *Chem. Phys. Lett.* 302, 485-488 (1999).

'Hot' $N+O_2$
Rate Constants
≤5000 K
Calculations

82246. Martinez, E., B. Cabanas, A. Aranda, P. Martin, A. Notario and S. Salgado, "Study on the NO_3 Radical Reactivity: Reactions with Cyclic Alkenes," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 5321-5327 (1999).

NO_3+*c*-Alkenes
Rate Constants
5 Molecules
T Dependences

82247. Canosa-Mas, C.E., M.D. King, L. McDonnell and R.P. Wayne, "An Experimental Study of the Gas Phase Reactions of the NO_3 Radical with Pent-1-ene, Hex-1-ene and Hept-1-ene," *Phys. Chem. Chem. Phys.* 1, 2681-2685 (1999).

$NO_3+C_5H_{10}$,C_6H_{12}
$NO_3+C_7H_{14}$
Rate Constants
Measurements

(82121) Rate Constants, Measurements

N_3H+OH
NH(a)+OH

82248. Guenther, J., B. Erbacher, D. Krankowsky and K. Mauersberger, "Pressure Dependence of Two Relative Ozone Formation Rate Coefficients," *Chem. Phys. Lett.* 306, 209-213 (1999).

$O+{}^{18}O^{18}O/O+O_2$
${}^{18}O+O_2/{}^{18}O+{}^{18}O^{18}O$
Relative
Rate Constants
Pressure
Dependences

82249. Fulle, D., H.F. Hamann and H. Hippler, "The Pressure and Temperature Dependence of the Recombination Reaction $HO+SO_2+M \rightarrow HOSO_2+M$," *Phys. Chem. Chem. Phys.* 1, 2695-2702 (1999).

$SO_2+OH+He$
Rate Constants
Fall-off Parameters

82250. Becerra, R., S. Boganov and R. Walsh, "A Gas Phase Kinetic Study of the Reaction of Silylene with Germane: Absolute Rate Constants, Temperature Dependence and Mechanism," *J. Chem. Soc., Faraday Trans.* 94, 3569-3572 (1998).

SiH_2+GeH_4
Rate Constant
Temperature
Dependence

37. PHOTOLYSIS/MPD

(See also Section 38 for Photolytic Product Distributions)

82251.	Langhals, H., J. Karolin and L.B-A. Johansson, "Spectroscopic Properties of New and Convenient Standards for Measuring Fluorescence Quantum Yields," *J. Chem. Soc., Faraday Trans.* 94, 2919-2922 (1998).	Actinometry Fluorescence Quantum Yield 3 New Standards
82252.	Gerasimov, I., J. Lei and P.J. Dagdigian, "Electronic Spectroscopy of the Al-CH_4/CD_4 Complex," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 5910-5917 (1999).	Al.CH_4+hν Al.CD_4+hν Al,AlH(A-X) Products Chemiluminescence
82253.	Skowronek, S., J.B. Jimenez and A. Gonzalez-Urena, "Spectroscopy and Dynamics of van der Waals Reactions: The Ba···FCH_3* Photofragmentation Channels," *Chem. Phys. Lett.* 303, 275-280 (1999).	Ba.FCH_3+hν Channels Probabilities
82254.	Farmanara, P., V. Stert, W. Radloff, S. Skowronek and A. Gonzalez-Urena, "Ultrafast Dynamics and Energetics of the Intracluster Harpooning Reaction in Ba···FCH_3," *Chem. Phys. Lett.* 304, 127-133 (1999).	Ba.FCH_3+hν 618 nm Excitation fs Reaction Time BaF* Product
82255.	Franks, K.J., H. Li, S.R. Kuy and W. Kong, "Photodissociation of ICN at 266 nm and BrCN at 230 nm Using Brute Force Orientation," *Chem. Phys. Lett.* 302, 151-156 (1999).	BrCN+hν ICN+hν Oriented Beams Product CN Effects
82256.	Ardelt, D., and F. Stuhl, "Two-Photon Photolysis of CF_3Cl at 10.5 eV: Determination of the Cl*/Cl Spin-Orbit Branching Ratio and the Formation of Electronically Excited CF_3*," *Chem. Phys. Lett.* 304, 323-328 (1999).	CF_3Cl+2hν CF_3*,Cl($^2P_{1/2,3/2}$) Fragment Distributions
82257.	Spasov, J.S., and J.I. Cline, "Scalar and Angular Correlations in CF_3NO Photodissociation: Statistical and Nonstatistical Channels," *J. Chem. Phys.* 110, 9568-9577 (1999).	CF_3NO+hν NO(J) Distribution Angular Correlations Channels
82258.	Melchior, A., H.M. Lambert, P.J. Dagdigian, I. Bar and S. Rosenwaks, "The Photodissociation of Ground and Vibrationally Excited Halogenated Alkanes," *Isr. J. Chem.* 37, 455-465 (1997).	CHF_2Cl,CH_3CF_2Cl+hν CH_3CFCl_2,CH_3Cl+hν Cl($^2P_{1/2,3/2}$),H Product Yields Vibrational Excitation Effects
82259.	Schwendner, P., C. Beck and R. Schinke, "Ladder Climbing and Multiphoton Dissociation of Polyatomic Molecules Excited with Short Pulses: Basic Theory and Applications to HCO," *Phys. Rev. A: At. Mol. Opt. Phys.* 58, 2203-2213 (1998).	IR MPA/MPD HCO Ladder Climbing Model

82260. Min, Z., T.-H. Wong and R. Bersohn, "Hydrogen Atom Release from Methyl Groups of Energized Molecules," *J. Chem. Phys.* 110, 9956-9960 (1999).

$CH_3Br+h\nu$
$(CH_3)_3N+h\nu$
$C_6F_5CH_3+h\nu$
H-Atom Formation
Mechanisms

82261. Samartzis, P.C., B.L.G. Bakker, D.H. Parker and T.N. Kitsopoulos, "Photoelectron and Photofragment Velocity Imaging Following the Excitation of CH_3I to the A-Band Using fs, ps and ns Laser Pulses," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 6106-6113 (1999).

MPD
CH_3I
fs,ps,ns
Laser Pulses
Product
Velocity Mapping

82262. Farmanara, P., V. Stert and W. Radloff, "Ultrafast Photodissociation of Methyl Nitrite Excited to the S_2 State," *Chem. Phys. Lett.* 303, 521-525 (1999).

$CH_3ONO+h\nu$
S_2 State
Dissociation Times
NO Fragment

(81985) Diamond Formation Method

IR MPD
$CH_4/Ar;CH_4/H_2$

82263. Chang, A.H.H., D.W. Hwang, X.-M. Yang, A.M. Mebel, S.H. Lin and Y.T. Lee, "Toward the Understanding of Ethylene Photodissociation: Theoretical Study of Energy Partition in Products and Rate Constants," *J. Chem. Phys.* 110, 10810-10820 (1999).

$C_2H_4+h\nu$
D-Isotopes
H,H_2 Product
Loss Energies
Channels
Calculations

82264. Thorson, G.M., C.M. Cheatum, M.J. Coffey and F.F. Crim, "Photofragment Energy Distributions and Dissociation Pathways in Dimethyl Sulfoxide," *J. Chem. Phys.* 110, 10843-10849 (1999).

$(CH_3)_2SO+h\nu$
CH_3,CH_3SO
Primary Products
Energies
Quantum Yields
Measurements

82265. Chang, J.-I., G.-c. Tseng, C.-K. Ni, J.-D. Huang and Y.-T. Chen, "Ionization and Emission Spectra of the Photofragments of Allene Excited at 193 nm," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 6063-6073 (1999).

$C_3H_4+nh\nu$
C^+,C_2^+,C_3^+
$C_3H_n^+$ Yields
C^*,C_2^*,CH^*
Spectral Emission
Mechanism

(81857) S_2, S_1-State Photodissociation fs Dynamics, State Lifetimes, Fragment Photoionization Probes, RRKM Analysis

$(CH_3)_2CO+h\nu$
$(CD_3)_2CO+h\nu$

82266. Kosmidis, C., J.G. Philis and P. Tzallas, "Laser Induced Ionization/Dissociation of Cyclopentanone in the 320-370 nm Region," *Phys. Chem. Chem. Phys.* 1, 2945-2948 (1999).

2PI/2PD
c-C_5H_8O
Channels
Jet Cooled Beam
Mass Analyzer

82267. Zhitneva, G.P., "A Comparison of the Infrared Multiphoton Dissociation of $C_3H_5C(CH_3)_3$ and $C_3H_5Ge(CH_3)_3$," *Chem. Phys. Lett.* 307, 379-384 (1999).

IR MPD
$C_3H_5C(CH_3)_3$
$C_3H_5Ge(CH_3)_3$
Yield
Comparisons

82268. Castillejo, M., S. Couris, E. Koudoumas and M. Martin, "Ionization and Fragmentation of Aromatic and Single-Bonded Hydrocarbons with 50 fs Laser Pulses at 800 nm," *Chem. Phys. Lett.* 308, 373-380 (1999).

MPD/MPI
Aromatic,Alkane
Hydrocarbons
fs Laser Pulses
Fragment
Ions

82269. Zhao, Y., and O. Kuhn, "Selective Infrared Laser Pulse Control of H and CO Branching in the Ground State Photodissociation of $HCo(CO)_4$: A Two-Dimensional Model Simulation," *Chem. Phys. Lett.* 302, 7-14 (1999).

IR MPD
$CoH(CO)_4$
Laser Control
Channels

82270. Roth, M., C. Maul, K.-H. Gericke, T. Senga and M. Kawasaki, "State and Energy Characterization of Fluorine Atoms in the A-Band Photodissociation of F_2," *Chem. Phys. Lett.* 305, 319-326 (1999).

$F_2+h\nu$
$F(^2P_{1/2,3/2})$
Products
REMPI Monitor

82271. Ferconi, M., J.J.V. Alvarez and S.T. Pantelides, "Selective Bond-Breaking in Molecules by Intense Infrared Radiation," *Chem. Phys. Lett.* 303, 57-64 (1999).

IR MPD
HCN
Bond Breaking
Mechanisms

82272. Tabayashi, K., J.-i. Aoyama, M. Matsui, T. Hino and K. Saito, "Dissociative Excitation of HCOOH by Single-Vacuum Ultraviolet and Two-Ultraviolet Photon," *J. Chem. Phys.* 110, 9547-9554 (1999).

$HCOOH+h\nu,2h\nu$
$OH(A),HCO,HCO_2^*$
Fragment Energies
Mechanisms

82273. Tachikawa, H., "Photodissociation Dynamics of Formyl Fluoride via the Triplet State Surface: A Direct ab Initio Dynamics Study," *Phys. Chem. Chem. Phys.* 1, 2675-2679 (1999).

$HFCO+h\nu$
Channels
Energy Barriers
Product Energies
Calculations

82274. Rottke, H., J. Ludwig and W. Sandner, "Two-Photon Dissociative Photoionization and Photodissociation of Single $H_2(B^1\Sigma_u^+,v=5)$ Rotational States," *J. Phys. B. At. Mol. Opt. Phys.* 30, 4049-4064 (1997).

2PD,2PI
$H_2(B,v=5)$
Fragment Energies
Distributions
Channels

82275. Kawata, I., H. Kono and Y. Fujimura, "Adiabatic and Diabatic Responses of H_2^+ to an Intense Femtosecond Laser Pulse: Dynamics of the Electronic and Nuclear Wavepacket," *J. Chem. Phys.* 110, 11152-11165 (1999).

Fs MPA/MPD
H_2^+
Theory

82276. Atabek, O., "Laser Induced Alignment Dynamics in Multiphoton Dissociation of H_2^+," *Int. J. Quantum Chem.* 65, 617-624 (1997).

IR ~ MPD
H_2^+
Fragment Angular Distributions
Calculations

82277. Dixon, R.N., D.W. Hwang, X.F. Yang, S. Harich, J.J. Lin and X. Yang, "Chemical 'Double Slits': Dynamical Interference of Photodissociation Pathways in Water," *Science* 285, 1249-1253 (1999).

$H_2O + h\nu$
121.6 nm
OH(v,J) Product Oscillations
2-Channel Interferences

(82048) (A-X) Photodissociation Cross Sections, Calculations

$H_2O + h\nu$

82278. Backhaus, P., B. Schmidt and M. Dantus, "Control of Photoassociation Yield: A Quantum-Dynamical Study of the Mercury System to Explore the Role of Pulse During from Nanoseconds to Femtoseconds," *Chem. Phys. Lett.* 306, 18-24 (1999).

$Hg + Hg + h\nu$
Photoassociation
Hg_2 Yields
Laser Pulse Duration Effects

82279. Durrani, S.M.A., and M. Ahmed, "Infrared Multiphoton Excitation and Dissociation Studies of SO_2," *Nuovo Cimento D: Condensed Matter, At. Mol. Chem. Phys.* 19, 1517-1523 (1997).

IR MPA/MPD
SO_2
Different CO_2 Laser Line Effects
Sulfur Formation

82280. Lyman, J.L., B.E. Newnam, T. Noda and H. Suzuki, "Enrichment of Silicon Isotopes with Infrared Free-Electron Laser Radiation," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 4227-4232 (1999).

IR MPD
Si_2F_6
Isotopic Enrichment Measurements

38. REACTION PRODUCT-ENERGY DISTRIBUTIONS

(See also Section 37 for Product Distributions and Section 40 for Theoretically Calculated Reaction Product Distributions)

82281. Pe'er, A., M. Shapiro and G.G. Balint-Kurti, "The Breaking of the Backward-Forward Symmetry in the Angular Distribution of m_j-Selected Photofragments," *J. Chem. Phys.* 110, 11928-11935 (1999).

Photofragments Angular Distributions
Theory

82282. Cooper, M.J., E. Wrede, A.J. Orr-Ewing and M.N.R. Ashfold, "Ion Imaging Studies of the $Br(^2P_J)$ Atomic Products Resulting from Br_2 Photolysis in the Wavelength Range 260-580 nm," *J. Chem. Soc., Faraday Trans.* 94, 2901-2907 (1998).

$Br(^2P_{1/2,3/2})$ Products
$Br_2 + h\nu$
Ion Imaging Method

82283.	Knepp, P.T., and S.H. Kable, "The Photodissociation Dynamics of CFBr Excited into the $A(^1A'')$ State," *J. Chem. Phys.* 110, 11789-11797 (1999).	$CF(X,v=0,\Lambda,J)$ Fragment Energies $CFBr+h\nu$ Photodissociation Dynamics
(82111)	Product Vibrational Distributions, $He(2^1S)+CO$ Penning Ionization	$CO^+(B,A,X)$
(82125)	Product Emission, $Ne(^3P_{0,2})+CO$, Penning Ionization	$CO^+(A,v,J)$
82284.	Brownsword, R.A., P. Schmiechen, H.-R. Volpp, H.P. Upadhyaya, Y.J. Jung and K.-H. Jung, "Chlorine Atom Formation Dynamics in the Dissociation of CH_3CF_2Cl(HCFC-142b) After Ultraviolet Laser Photoexcitation," *J. Chem. Phys.* 110, 11823-11829 (1999).	$Cl(^2P_{1/2,3/2})$ Product Energies $CH_3CF_2Cl+h\nu$ Mechanism
82285.	Regan, P.M., S.R. Langford, D. Ascenzi, P.A. Cook, A.J. Orr-Ewing and M.N.R. Ashfold, "Spin-Orbit Branching in $Cl(^2P)$ Atoms Produced by Ultraviolet Photodissociation of HCl," *Phys. Chem. Chem. Phys.* 1, 3247-3251 (1999).	$Cl(^2P_{1/2,3/2})$ Product Branching $HCl+h\nu$ Jet Cooled
82286.	Rakitzis, T.P., S.A. Kandel, A.J. Alexander, Z.H. Kim and R.N. Zare, "Photofragment Helicity Caused by Matter-Wave Interference from Multiple Dissociative States," *Science* 281, 1346-1349 (1998).	$^{35,37}Cl$ Oriented Fragments $ICl+h\nu$ Linearly Polarized Light
(82240)	'Hot' $H+D_2$ Crossed Beam, Cross Sections	D Product Energies
82287.	Lai, L.-H., Y.T. Hsu and K. Liu, "On the H-Atom Formation after Lyman-α Excitation of CHF_2Cl," *Chem. Phys. Lett.* 307, 385-390 (1999).	H Fragment Velocities $CHF_2Cl+h\nu$ Channels
(81861)	$D_2^++H_2$ Product Ions, Mechanism	H*,D*
(81877)	Product, Fragment Energies, $OH^+(v=0)+e^-$, Mechanism	$H(n=2)$
82288.	Yokoyama, A., and T. Takayanagi, "Rotational and Vibrational Energy Distributions of HCl Produced by Three- and Four-Center Eliminations of HCl from Halogenated Ethanes," *Chem. Phys. Lett.* 307, 48-54 (1999).	$HCl(v,J)$ Product Energies CF_3CHFCl CH_3CF_2Cl Elimination Mechanisms
82289.	Kennedy, S., K. Dharmesena, S. Moser, M. Auzinsh and N.E. Shafer-Ray, "A Method to Obtain meV Collision Energy Resolution in Scattering Studies: Application to the $H+D_2\rightarrow HD(v'=0,j')+D(\theta_{rel}<80°)$ Reaction at $E_{rel}=1.275(\pm0.011)$ eV," *Chem. Phys.* 244, 449-469 (1999).	$HD(v=0,J)$ Product Yield $H+D_2$ Measurements

82290.	Baer, M., M. Faubel, B. Martinez-Haya, L. Rusin, U. Tappe and J.P. Toennies, "Rotationally Resolved Differential Scattering Cross Sections for the Reaction $F+para\text{-}H_2$ $(v=0,j=0) \rightarrow HF(v'=2,3,j')+H$," *J. Chem. Phys.* 110, 10231-10234 (1999).	HF(v,J) Product Distributions $F+H_2$ Measurements
82291.	Liu, D.-K., and K.-C. Lin, "Reaction Dynamics of Mg(3s4s $^1S_0$) with H_2: Interference of the MgH Product Contribution from the Lower Mg(3s3p $^1P_1$) State," *Chem. Phys. Lett.* 304, 336-342 (1999).	MgH(v=0,1,N) Product Distribution $Mg(^1S_0)+H_2$ Major Role
82292.	Shin, S.K., H.L. Kim and C.R. Park, "Photodissociation Dynamics of *tert*-Butyl Hydroperoxide at 193 nm," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 4150-4154 (1999).	OH(X,v,J,T) Product Energy Distribution $C_4H_9OOH+h\nu$ Dynamics
82293.	Yoon, M.-C., Y.S. Choi and S.K. Kim, "Photodissociation Dynamics of Acetylacetone: The OH Product State Distribution," *J. Chem. Phys.* 110, 11850-11855 (1999).	OH(X,v,J) Product Energies $CH_2(COCH_3)_2+h\nu$ Mechanism
82294.	Tsuboi, S., T. Sawai, H. Ohoyama and T. Kasai, "Nascent Internal-State Distribution of Product $OH(A^2\Sigma)$ Observed in a Crossed Beam Reaction of Hot H-Atom with N_2O," *Bull. Chem. Soc. Jpn .* 71, 1581-1585 (1998).	OH(A,v,J) Product Energy Distributions 'Hot' $H+N_2O$ Measurements
82295.	Brouard, M., I. Burak, S.D. Gatenby, D. Hart and D. Minayev, "The $H+N_2O \rightarrow OH(^2\Pi_{3/2},v',N')+N_2$ Reaction at 1.5 eV: New Evidence for Two Microscopic Mechanisms," *J. Chem. Phys.* 110, 11335-11345 (1999).	OH(X,v,N) Product Energy Distributions 'Hot' $H+N_2O$ Dual Mechanisms
(82130)	Product Distributions, $O(^1D_2)+H_2(v=0,J)$, $O(^1D_2)$ from Polarized N_2O Dissociation, Measurements, Calculations	OH(X,v,N,f)
82296.	O'Keeffe, P., T. Ridley, K.P. Lawley, R.R.J. Maier and R.J. Donovan, "Kinetic Energy Analysis of $O(^3P_0)$ and $O_2(b^1\Sigma_g^+)$ Fragments Produced by Photolysis of Ozone in the Huggins Bands," *J. Chem. Phys.* 110, 10803-10809 (1999).	$O_2(b,v=0),O(^3P_0)$ Velocities $O_3+h\nu$ (351.4,322.6 nm) Mechanisms
82297.	Teule, J.M., M.H.M. Janssen, J. Bulthuis and S. Stolte, "Laser Induced Fluorescence Studies of Excited Sr Reactions: II. $Sr(^3P_1)+CH_3F$, C_2H_5F, $C_2H_4F_2$," *J. Chem. Phys.* 110, 10792-10802 (1999).	SrF(X,v,J) Product Energy Distributions $Sr(^3P_1)+RF,RF_2$

39. UNIMOLECULAR PROCESSES

(See also Section 36 for Unimolecular Rate Constants and Section 40 for Reaction Dynamics)

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(82457)	Isomerization Barrier, v,J Levels, Structural Calculations, AlO^+ Electronic Structure	$AlOH^+$,$HAlO^+$
82299.	Keller, H.-M., and R. Schinke, "The Unimolecular Dissociation of HCO. IV. Variational Calculation of Siegert States," *J. Chem. Phys.* 110, 9887-9897 (1999).	Unimolecular Dissociation HCO DCO Resonance States Calculations
82300.	Orel, A.E., and O. Kuhn, "Cartesian Reaction Surface Analysis of the CH_2I_2 Ground State Isomerization," *Chem. Phys. Lett.* 304, 285-292 (1999).	Isomerization CH_2I_2 P.E. Surface
82301.	Shapley, W.A., and G.B. Bacskay, "Ab Initio Quantum Chemical Studies of the Formaldiminoxy (CH_2NO) Radical. I. Isomerization Reactions," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 4505-4513 (1999).	Isomerizations CH_2NO P.E. Surface Isomers ΔH_f(NH_2CO,CH_2NO) Channels
(82527)	Unimolecular Dissociation, Rate Constants, ΔH_f, D, Measurements, Calculations	CH_3SO_2,CH_3OSO
82302.	Schork, R., and H. Koppel, "Ab Initio Quantum Dynamical Study of the Vinylidene-Acetylene Isomerization," *Theor. Chem. Acc.* 100, 204-211 (1998).	Isomerization CCH_2/C_2H_2 Dynamics CCH_2 Lifetime Calculations
82303.	Jursic, B.S., "Complete Basis Set ab Initio Computational Exploration of the Lowest Energy, Unimolecular, Triplet Potential Energy Surface for Triplet Oxygen Atom Assisted Acetylene Rearrangement into Vinylidene," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 5773-5783 (1999).	Unimolecular Rearrangement C_2H_2/CCH_2 O-Atom Assisted Mechanism

82304.	Pena-Gallego, A., E. Martinez-Nunez and S.A. Vazquez, "Nonstatistical Effects in the Unimolecular Dissociation of the Acetyl Radical," *J. Chem. Phys.* 110, 11323-11334 (1999).	Unimolecular Dissociation CH_3CO IVR non-RRKM Calculations
82305.	Martell, J.M., H. Yu and J.D. Goddard, "Molecular Decompositions of Acetaldehyde and Formamide: Theoretical Studies Using Hartree-Fock, Moller-Plesset and Density Functional Theories," *Mol. Phys.* 92, 497-502 (1997).	Unimolecular Dissociation CH_3CHO NH_2CHO Channels Energetics Calculations
82306.	Caralp, F., P. Devolder, C. Fittschen, N. Gomez, H. Hippler, R. Mereau, M.T. Rayez, F. Striebel and B. Viskolcz, "The Thermal Unimolecular Decomposition Rate Constants of Ethoxy Radicals," *Phys. Chem. Chem. Phys.* 1, 2935-2944 (1999).	Unimolecular Dissociation C_2H_5O+M Rate Constants Fall-off Parameters
82307.	Kim, D.Y., J.C. Choe and M.S. Kim, "Quantum Mechanical Tunneling in the Unimolecular Dissociation of the Propargyl Bromide Molecular Ion," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 4602-4608 (1999).	Unimolecular Dissociation $CHCCH_2Br^+$ Isomers $C_3H_3^+$ Product Calculations
(82409)	MPI, Isomerization, Fragment Ions, Mechanisms	$(CH_3)_2CO$
82308.	Ceno, M.D., A. Gonzalez-Lafont, J.M. Lluch and J. Bertran, "Theoretical Study of the Unimolecular Dissociation of the Acetone Cation Radical," *Mol. Phys.* 92, 393-398 (1997).	Unimolecular Dissociation $(CH_3)_2CO^+$ Channels Mechanism
82309.	Schroeter, K., D. Schroder and H. Schwarz, "Structures of the $C_8H_6^+$ Cation Formed upon Loss of Acetylene from Ionized Naphthalene," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 4174-4181 (1999).	Unimolecular Dissociation $C_{10}H_8^+$ C_2H_2 Loss $C_8H_6^+$ Product Structure
82310.	Zyrianov, M., A. Sanov, T. Droz-Georget and H. Reisler, "Photoinitiated Decomposition of HNCO Near the H+NCO Threshold: Centrifugal Barriers and Channel Competition," *J. Chem. Phys.* 110, 10774-10783 (1999).	Unimolecular/ S_0-T_1 Transfer $HNCO+h\nu$ Dissociation Channels Efficiencies

82311. Lin, C.-L., M.-D. Su and S.-Y. Chu, "A Theoretical Study of Dissociation Pathways of HICO," *Chem. Phys. Lett.* 308, 142-146 (1999).

Unimolecular
Dissociation
ICHO
Channels
Energies
Calculations

82312. Petrie, S., "Trends in M(CN) Isomerism: A Computational Study of Monocyanides of the Main-Group Third Row Atoms," *Phys. Chem. Chem. Phys.* 1, 2897-2905 (1999).

Isomerization
MCN/MNC
P.E. Surfaces
Neutrals,Cations
M=K,Ca,Ga,
Ge,As,Se,Br
Calculations

40. CHEMICAL DYNAMICS - THEORY

(See also Section 37 for Photodissociation Dynamics)

82313. Reignier, D., and T. Stoecklin, "Comparison of the Spin-Orbit Selectivity of Reactions Involving Atoms in a ^2P or ^3P State and a Linear Molecule in a Π or Σ State at Very Low Temperature," *Chem. Phys. Lett.* 303, 576-582 (1999).

Reaction Dynamics
$^2P, ^3P + ^2\Pi, ^2\Sigma, ^3\Sigma$
Rate Constants
Spin-Orbit Selectivity
Low Temperatures

82314. Desouter-Lecomte, M., and X. Chapuisat, "Quantum-Mechanical Statistical Theories for Chemical Reactivity: Overlapping Resonances," *Phys. Chem. Chem. Phys.* 1, 2635-2648 (1999).

Reaction Dynamics
Chemical Reactivity
TST Rate Constant
Saturation
Resolution

82315. Marquez, M., F. Mari and C.A. Gonzalez, "Ab Initio Study of the Reactions between a Series of Substituted Singlet Nitrenium Ions and Water," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 6191-6199 (1999).

Reaction Dynamics
$^1RNH + H_2O$
$R = CH_3$,CN,
Cl,F,H
Channels
Energies

82316. Takahashi, H., T. Kasai, K. Yamaguchi and H.H. Loesch, "Three Dimensional Wavepacket Simulation on the H Atom Scattering for the Full Reaction of $CF_3H + Ar(^3P) \rightarrow CF_3{}^* + H + Ar$," *Isr. J. Chem.* 37, 359-365 (1997).

Reaction Dynamics
$Ar(^3P) + CHF_3$
Steric Effects
$CF_3{}^*$ Product Channel

82317. Fang, W.-H., and S.D. Peyerimhoff, "Theoretical Studies on Mechanisms of the Insertion of Boron into Methane and Its Consequent Reactions," *Mol. Phys.* 93, 329-339 (1998).

Reaction Dynamics
$B + CH_4$
Insertion
Energetics
Channels

82318. Alberti, M., X. Gimenez, A. Aguilar and A.G. Urena, "Angular Momenta Correlation in Kinematically Constrained Reactions," II. Application to the $B+OH \rightarrow BO+H$ System," *Mol. Phys.* 93, 389-397 (1998).

Reaction Dynamics
$B+OH$
Angular Momentum Correlations

82319. Volobuev, Y.L., M.D. Hack and D.G. Truhlar, "Are Semiclassical Methods Accurate for Electronically Nonadiabatic Transitions between Weakly Coupled Potential Energy Surfaces?," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 6225-6233 (1999).

Reaction Dynamics
$Br(^2P_{1/2})+H_2$
Probabilities
4 Models Tested
Accuracies

82320. Hwang, D.-Y., A.M. Mebel and B.-C. Wang, "Ab Initio Study of the Addition of Atomic Carbon with Water," *Chem. Phys.* 244, 143-149 (1999).

Reaction Dynamics
$C+H_2O$
$C(^1D)+H_2O$
P.E. Surfaces
Channels
Energies

82321. Ochsenfeld, C., R.I. Kaiser, Y.T. Lee and M. Head-Gordon, "Coupled-Cluster ab Initio Investigation of Singlet/Triplet CH_2S Isomers and the Reaction of Atomic Carbon with Hydrogen Sulfide to HCS/HSC," *J. Chem. Phys.* 110, 9982-9988 (1999).

Reaction Dynamics
$C+H_2S$
HCS/HSC
Product Channels
Mechanism

82322. Gonzalez, A.I., A. Luna and M. Yanez, "High Level ab Initio Calculations on the Gas Phase Reactions between $C^+(^2P)$ and Formic Acid," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 4543-4552 (1999).

Reaction Dynamics
$C^++HCOOH$
P.E. Surface
Channels
Products

82323. Vereecken, L., and J. Peeters, "Detailed Microvariational RRKM Master Equation Analysis of the Product Distribution of the $C_2H_2+CH(X^2\Pi)$ Reaction over Extended Temperature and Pressure Ranges," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 5523-5533 (1999).

Reaction Dynamics
$CH+C_2H_2$
RRKM Analysis
Product Distributions
T,P Dependences

82324. Wang, Z.-X., and M.-B. Huang, "Ylide-like Addition Complexes in Insertion Reactions of CH with PH_3 and H_2S," *Chem. Commun.* 905-906 (1998).

Reaction Dynamics
$CH+H_2S$
$CH+PH_3$
Insertion
Energies

82325. Wang, B., H. Hou and Y. Gu, "A New Mechanism for the $CH(X^2\Pi)+NO(X^2\Pi) \rightarrow CO(X^1\Sigma^+)+NH(X^3\Sigma^-)$ Reaction on the Triplet Surface," *Chem. Phys. Lett.* 305, 163-168 (1999).

Reaction Dynamics
$CH+NO$
P.E. Surface
4-Center Transition
Mechanism

82326. Cui, Q., K. Morokuma, J.M. Bowman and S.J. Klippenstein, "The Spin-Forbidden Reaction $CH(^2\Pi)+N_2 \rightarrow HCN+N(^4S)$ Revisited. II. Nonadiabatic Transition State Theory and Application," *J. Chem. Phys.* 110, 9469-9482 (1999).
Reaction Dynamics
$CH+N_2$
Rate Constant
Discrepancies

82327. Wang, B., H. Hou and Y. Gu, "Ab Initio Studies of the Reaction of $O(^3P)$ with CHClF Radical," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 5075-5079 (1999).
Reaction Dynamics
CHClF+O
Channels
Branching Ratio
Rate Constants

82328. Sakai, S., "Theoretical Model for the Reaction Mechanisms of Singlet Carbene Analogs into Unsaturated Hydrocarbon and the Origin of the Activation Barrier," *Int. J. Quantum Chem.* 70, 291-302 (1998).
Reaction Dynamics
$CH_2, SiH_2+C_2H_4$
$GeH_2, SnH_2+C_2H_4$
$CF_2, SiF_2+C_2H_4$
$GeF_2, SnF_2+C_2H_4$
P.E. Surfaces
$\Delta H_{Reaction}$

82329. Shapley, W.A., and G.B. Bacskay, "Ab Initio Quantum Chemical Study of the Formation, Decomposition and Isomerization of the Formaldiminoxy Radical, CH_2NO: Comparison of the Gaussian-2 and CASPT2 Techniques in the Calculation of Potential Energy Surfaces," *Theor. Chem. Acc.* 100, 212-221 (1998).
Reaction Dynamics
$^3CH_2+NO$
CH_2NO Formation
Isomerization
Dissociation
Channels

82330. Wang, B., H. Hou and Y. Gu, "Ab Initio Potential Energy Surface for the Reaction of $O(^3P)$ with CH_2F," *Chem. Phys. Lett.* 304, 278-284 (1999).
Reaction Dynamics
CH_2F+O
P.E. Surface
Channels
Rate Constant

82331. Shapley, W.A., and G.B. Bacskay, "Ab Initio Quantum Chemical Studies of the Formaldiminoxy (CH_2NO) Radical. II. Dissociation Reactions," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 4514-4524 (1999).
Reaction Dynamics
CH_2NO
Dissociation
Product Channels
Energies

82332. Nguyen, M.T., T.L. Nguyen and H.T. Le, "Theoretical Study of Dithioformic Acid, Dithiohydroxy Carbene and Their Radical Cations: Unimolecular and Assisted Rearrangements," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 5758-5765 (1999).
Reaction Dynamics
$HCSSH, HCSSH^+$
$C(SH)_2, C(SH)_2^+$
P.E. Surfaces
Unimolecular
Dissociations
ΔH_f, IP, PA

82333. Naroznik, M., "Recombination of Radicals in the High Pressure and High Temperature Limit. I. Reaction CH_3+CH_3," *J. Chem. Soc., Faraday Trans.* 94, 2531-2539 (1998).
Reaction Dynamics
CH_3+CH_3
High Pressures
T>200 K
Rate Constant
Calculations

82334. Naroznik, M., and J. Niedzielski, "Recombination of Radicals in the High Pressure and High Temperature Limit. II. Reaction CH_3+H," *J. Chem. Soc., Faraday Trans.* 94, 2541-2547 (1998).

Reaction Dynamics
CH_3+H
High Pressures
T>200 K
Rate Constant
Calculations

82335. Kurosaki, Y., and T. Takayanagi, "Theoretical Study of an Isotope Effect on Rate Constants for the $CH_3+H_2 \rightarrow CH_4+H$ and $CD_3+H_2 \rightarrow CD_3H+H$ Reactions Using Variational Transition State Theory and the Multidimensional Semiclassical Tunneling Method," *J. Chem. Phys.* 110, 10830-10842 (1999).

Reaction Dynamics
CH_3+H_2
CD_3+H_2
Rate Constants
Barrier Heights
Isotope Effect

82336. Le, T.N., L.T. Nguyen and M.T. Nguyen, "Theoretical Study of the CH_3+NS and Related Reactions: Mechanism of HCN Formation," *Mol. Phys.* 96, 1817-1822 (1999).

Reaction Dynamics
CH_3+NS
HCN Formation
P.E. Surface
Channels
ΔH_f(Isomers)

82337. Eckert, F., and H.-J. Werner, "Reaction Path Following by Quadratic Steepest Descent," *Theor. Chem. Acc.* 100, 21-30 (1998).

Reaction Dynamics
Path Algorithm
CH_3O/CH_2O
C_2H_5F/C_2H_4+HF
HCN/HNC
Method

82338. Chuang, Y.-Y., M.L. Radhakrishnan, P.L. Fast, C.J. Cramer and D.G. Truhlar, "Direct Dynamics for Free Radical Kinetics in Solution: Solvent Effect on Rate Constant for the Reaction of Methanol with Atomic Hydrogen," *J. Phys. Chem. A. Mol., Spectrosc.,* 103, 4893-4909 (1999).

Reaction Dynamics
CH_3OH+H
Gas/Liquid Phases
Rate Constants
D Effects

82339. Lacombe, S., M. Loudet, H. Cardy and A. Dargelos, "The Thiyl Peroxyl Radical: Formation and Ultraviolet Spectrum: A Multiconfigurational ab Initio Study," *Chem. Phys.* 244, 175-183 (1999).

Reaction Dynamics
CH_3S+O_2
Energy Barrier
CH_3SO_2 Energy
Electronic Structure
UV Spectrum

82340. Duncan, W.T., R.L. Bell and T.N. Truong, "THERATE: Program for ab Initio Direct Dynamics Calculations of Thermal and Vibrational-State-Selected Rate Constants," *J. Computat. Chem.* 19, 1039-1052 (1998).

Reaction Dynamics
Rate Constants
VTST/Tunneling
Program
CH_4+H
Model Example

82341. Resende, S.M., J.R. Pliego Jr and W.B. De Almeida, "Free Radical Mechanism of the Cl_2 Addition to Acetylene," *J. Chem. Soc., Faraday Trans.* 94, 2895-2900 (1998).

Reaction Dynamics
C_2H_2+Cl,Cl_2
$C_2H_2Cl+Cl_2$
$C_2H_2Cl+C_2H_2$
Rate Constants
Mechanism
Products

82342. Nguyen, H.M.T., R. Sumathi and M.T. Nguyen, "Mechanism and Kinetics of the Reaction of Acetylene and Nitric Oxide," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 5015-5022 (1999).

Reaction Dynamics
C_2H_2+NO
P.E. Surface
Channels
Rate Constants
HCO+HCN
Products

82343. Laskin, A., and H. Wang, "On Initiation Reactions of Acetylene Oxidation in Shock Tubes: A Quantum Mechanical and Kinetic Modeling Study," *Chem. Phys. Lett.* 303, 43-49 (1999).

Reaction Dynamics
C_2H_2/O_2
Isomerization
Initiation
Shock Tube
Mechanism

82344. Villa, J., J.C. Corchado, A. Gonzalez-Lafont, J.M. Lluch and D.G. Truhlar, "Variational Transition State Theory with Optimized Orientation of the Dividing Surface and Semiclassical Tunneling Calculations for Deuterium and Muonium Kinetic Isotope Effects in the Free Radical Association Reaction $H+C_2H_4 \rightarrow C_2H_5$," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 5061-5074 (1999).

Reaction Dynamics
C_2H_4+H
VTST
Isotope Effects

82345. Alvarez-Idaboy, J.R., I. Diaz-Acosta and A. Vivier-Bunge, "Energetics of Mechanism of OH/Propene Reaction at Low Pressures in Inert Atmosphere," *J. Computat. Chem.* 19, 811-819 (1998).

Reaction Dynamics
C_2H_4+OH
C_3H_6+OH
Channels
Energies

82346. Chiu, S.-W., K.-C. Lau and W.-K. Li, "An ab Initio Study of the $[C_2H_5O^-]$ Potential Energy Surface and the Fragmentation Pathways of the Ethoxide Anion," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 6003-6008 (1999).

Reaction Dynamics
$C_2H_5O^-$
P.E. Surface
Isomers
ΔH_f
Fragmentation
Channels

82347. Resende, S.M., and W.B. De Almeida, "Mechanism of the Atmospheric Reaction between the Radical CH_3SCH_2 and O_2," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 4191-4195 (1999).

Reaction Dynamics
$CH_3SCH_2+O_2$
Energy Barrier
$\Delta H_f(CH_3SCH_2)$

82348.	Resende, S.M., and W.B. De Almeida, "Thermodynamical Analysis of the Atmospheric Fate of the $CH_3SCH_2O_2$ Radical," *Phys. Chem. Chem. Phys.* 1, 2953-2959 (1999).	Reaction Dynamics $CH_3SCH_2O_2 + M$ M = 9 Reactants Rate Constants $\Delta H_f(CH_3O_2, CH_3SO)$ $\Delta H_f(CH_3SO_2, CH_3SO_3)$ $\Delta H_f(CH_3SCH_2O)$
82349.	Sobolewski, A.L., and W. Domcke, "Photophysics of Malonaldehyde: An ab Initio Study," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 4494-4504 (1999).	Reaction Dynamics $CH_2(CHO)_2$ Proton Transfer H-Transfer Low-lying States Mechanisms
82350.	Ben-Nun, M., and T.J. Martinez, "Semiclassical Tunneling Rates from ab Initio Molecular Dynamics," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 6055-6059 (1999).	Reaction Dynamics $CH_2(CHO)_2$ Tunneling Rates Method
82351.	Chan, W.-T., I.P. Hamilton and H.O. Pritchard, "Self-Abstraction in Aliphatic Hydroperoxyl Radicals," *J. Chem. Soc., Faraday Trans.* 94, 2303-2306 (1998).	Reaction Dynamics RO_2 R = Alkyl Intramolecular H-Atom Transfer Activation Energies Rate Constants
82352.	Davis, W.M., S.M. Heck and H.O. Pritchard, "Theoretical Study of Benzyl Radical Reactivity in Combustion Systems," *J. Chem. Soc., Faraday Trans.* 94, 2725-2728 (1998).	Reaction Dynamics $C_6H_5CH_2 + HO_2$ OH Source Rate Constants Ignition Role
82353.	Bauschlicher Jr, C.W., "The Reaction of Polycyclic Aromatic Hydrocarbon Cations with Hydrogen Atoms: The Astrophysical Implications [*Astrophys. J.* 509, L125-L127 (1998)]," *ibid.* 517, L67 (1999).	Reaction Dynamics $C_{10}H_8D^+ + H$ Energies,Barriers Erratum
82354.	Aihara, J.-i., "Why are Some Polycyclic Aromatic Hydrocarbons Extremely Reactive?," *Phys. Chem. Chem. Phys.* 1, 3193-3197 (1999).	Reaction Dynamics PAHS Relative Reactivities Theoretical Basis
82355.	Luna-Garcia, H., S. Castillo and A. Ramirez-Solis, "Ab Initio Studies of the Reactions of $M(^1S, ^3P$ and $^1P)$ with SiH_4, (M = Cd,Hg)," *J. Chem. Phys.* 110, 11315-11322 (1999).	Reaction Dynamics $Cd(^{1,3}P, ^1S_0) + SiH_4$ $Hg(^{1,3}P, ^1S_0) + SiH_4$ P.E. Surfaces Energy Barriers

82356. Wang, H., and W.H. Miller, "Analytic Continuation of Real-Time Correlation Functions to Obtain Thermal Rate Constants for Chemical Reaction," *Chem. Phys. Lett.* 307, 463-468 (1999).

Reaction Dynamics
$Cl+H_2$
Rate Constant
Correlation
Function Method

82357. Aoiz, F.J., L. Banares and V.J. Herrero, "Recent Results from Quasiclassical Trajectory Computations of Elementary Chemical Reactions," *J. Chem. Soc., Faraday Trans.* 94, 2483-2500 (1998).

Reaction Dynamics
$Cl,F,H+H_2$
$O(^1D)+H_2$
Rate Constants
Method Accuracies

82358. Schmatz, S., and D.C. Clary, "Quantum Scattering Calculations on the S_N2 Reaction $Cl^-+CH_3Br \rightarrow ClCH_3+Br^-$," *J. Chem. Phys.* 110, 9483-9491 (1999).

Reaction Dynamics
$Cl^-+CH_3Br(v,J)$
Rate Constant
ΔJ Propensity

82359. Okuno, Y., "Effects of Reaction Path Curvature on Reaction Dynamics and Rates: Reaction Path Hamiltonian Calculations for Gas Phase S_N2 Reaction Cl^-+CH_3Cl," *Int. J. Quantum Chem.* 68, 261-271 (1998).

Reaction Dynamics
Cl^-+CH_3Cl
Cl Exchange
P.E. Surface
Path Curvature

82360. Botschwina, P., "The Saddle Point of the Nucleophilic Substitution Reaction Cl^-+CH_3Cl: Results of Large-Scale Coupled Cluster Calculations," *Theor. Chem. Acc.* 99, 426-428 (1998).

Reaction Dynamics
Cl^-+CH_3Cl
Atom Exchange
Energy Barrier

82361. Nakao, Y., T. Taketsugu and K. Hirao, "Theoretical Study of Ammonia Activation by Sc^+, Ni^+ and Cu^+," *J. Chem. Phys.* 110, 10863-10873 (1999).

Reaction Dynamics
$Cu^+(^1S)+NH_3$
$Ni^+(^2D)+NH_3$
$Sc^+(^{1,3}D)+NH_3$
P.E. Surface
Stationary Points
Binding Energies

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Reaction Dynamics
$F+D_2$
Spin-Orbit
Corrections
Negligible Effects

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Reaction Dynamics
$F+D_2(v=0,J=0\text{-}2)$
DF(v,J) Product
Cross Sections
Calculations

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Reaction Dynamics
$F+H_2$
P.E. Surface
State-to-State
Probabilities

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Reaction Dynamics
$F+H_2S$
$F+D_2S$
Product v,J
3-Center
P.E. Surface

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Reaction Dynamics
F^-+CH_3Cl
P.E. Surface
Mechanism

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Reaction Dynamics
FCO+NO
Mechanism
FNO,CO
Products

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Reaction Dynamics
H+HCl
H+DCl
Channels
Cross Sections
Reactant v,J
Effects

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Reaction Dynamics
$H+H_2(v,J)$
Cross Sections
Dissociation Channel

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Reaction Dynamics
H_2+H_2
Exchange
Dissociation
Mechanisms

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Reaction Dynamics
$H_2(v,J)+He$
Probabilities
Rotational
Effects

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Reaction Dynamics
Saddle Point
Search Algorithm
HCN/HNC
Example

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Reaction Dynamics
2 HCOOH
$HCOOH + H_2O$
Dissociation
Channels
Energy Barriers
Rate Constants

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Reaction Dynamics
H_2O_2
P.E. Surface
$H_2 + O_2$/OH + OH/
$H + HO_2$/O + H_2O
Alternate Channels
Rate Constants

(82118) P.E. Surfaces, Conical Intersection, Quenching Dynamics, Calculations
$Li(^2P) + H_2$

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Reaction Dynamics
Li,Na + Li_2(v)
Li + Na_2(v)
Dissociative
Cross Sections

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Reaction Dynamics
$N + N_2$(v,J)
Dissociation
Cross Sections

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Reaction Dynamics
$NH + CH_4, C_2H_6$
Rate Constants
Paths
Energy Barriers

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Reaction Dynamics
$NS + NH_2$
P.E. Surfaces
Channels
$\Delta H_f(N_2H_2S)$
Isomers

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Reaction Dynamics
$NH_2+C_2H_6$
NH_3 Channel
Rate Constants

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Reaction Dynamics
NH_2+NH_2
Rate Constant
T Dependence
Energy Barrier

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Reaction Dynamics
$N_2^+ + O_2$
Channels
Energies

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Reaction Dynamics
N_2O
Predissociation
Spin-Forbidden
Channel
P.E. Surfaces

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Reaction Dynamics
O+HCl(v,J)
Probabilities
OH Product Energies

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Reaction Dynamics
$OH+O_2(v)$
HO_2 Product
Energy Distributions
Cross Sections

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Reaction Dynamics
$^1O_2+C_2H_4$
Transition States
Stabilities
Mechanism

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Reaction Dynamics
$P^+ + NH_3$
Rate Constants
Channels
Branching Ratio

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Reaction Dynamics
$S^+ + C_2H_2$
Channels
Energies

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(81783)	CO/O_2/Pt, Suppression, Feedback Concept	Kinetic Oscillations
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82393.	Cheema, S.A., K.A. Holbrook, G.A. Oldershaw, D.P. Starkey and R.W. Walker, "The Effect of Oxygen Pressure on the Tropospheric Oxidation of Diethyl Ether, H-Atom Elimination from the 1-Ethoxyethoxy Radical," *Phys. Chem. Chem. Phys.* 1, 3243-3245 (1999).	$(C_2H_5)_2O/O_2$ Product Yields Mechanism

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(81773) Solar Oven, Zn Formation Yields | ZnO(s) Dissociation

42. LASERS/INDUCED EFFECTS/MPI

(See also Section 26 for REMPI Spectra)

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(82269)	IR MPD, Laser Control, Channels	$CoH(CO)_4$
82404.	Dion, C.M., A.D. Bandrauk, O. Atabek, A. Keller, H. Umeda and Y. Fujimura, "Two-Frequency Infrared Laser Orientation of Polar Molecules: Numerical Simulations for HCN," *Chem. Phys. Lett.* 302, 215-223 (1999).	IR Laser Orientation HCN Method
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(82268) MPD/MPI, fs Laser Pulses, Fragment Ions — Aromatic, Alkane Hydrocarbons

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MPI
$(CH_3)_2CO$
Fragment Ions
Isomerization
Mechanisms

(82266) 2PI/2PD, Channels, Jet Cooled Beam, Mass Analyzer — c-C_5H_8O

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fs MPI
C_6H_6, $C_{10}H_8$
$C_{14}H_{10}$
Yields
Model

(82270) REMPI Product Monitor, $F_2+h\nu$ — $F(^2P_{1/2,3/2})$

(82274) 2 PD, 2PI, Fragment Energies, Distributions, Channels — $H_2(B,v=5)$

(82168) New Method, Monitoring Assessment — REMPI, Hg

43. P.E. CURVES/SURFACES/ENERGY LEVELS

(See also Section 26 for Spectral Aspects, Section 40 for Surface Dynamics and Section 44 for Structure Calculation Surfaces)

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v,J Energy Levels
CH_2N, CH_2S
Calculation
Code

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Vibrational
Energy Levels
$CS_2(X)$
$\leq$20,000 cm^{-1}
Dispersed
Fluorescence
Measurements

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Co^+
Energy Levels
FT Spectrum
Assignments

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Energy Spacings
$Cs(^2P_{1/2}$-$^2S_{1/2})$
$Cs(^2P_{1/2}, F_4/F_3)$
Measurements

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Vibrational Energy Levels
HN_3,DN_3
P.E. Functions
Calculations

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v,J Energy Levels
Triatomics
Calculation Method
H_2O Testing

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v,J Energy Levels
NCS(X)
Renner-Teller
Calculations
(B,A) Conical Intersection

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Vibrational Energy Levels
NH_3
Calculation Method

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v,J Energy Levels
$(O_2)_2$
v≤25 Bound States
D_0
Calculations

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v,J Energy Levels
$(O_2(a))_2$
(v=0,0),(1,0) Dimers
Bound States
D_0

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Vibrational Energy Levels
SH(A).Rg
SD(A).Rg
Rg=Ar,Kr
Calculations

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v,J Energy Levels
Si_3(X)
Simulated Spectrum

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P.E. Surfaces
D_e
Gaussian-3
Method

(82312) Isomerization P.E. Surfaces, M = K, Ca, Ga, Ge, As, Se, Br, Calculations

MCN/MNC
MCN^+/MNC^+

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P.E. Curves
$ArCl^-$
$ArCl(X,I_{3/2},II_{1/2})$
ZEKE Spectra
Constants
Well Depths

82425. Ehara, M., M. Nakata, H. Kou, K. Yasuda and H. Nakatsuji, "Direct Determination of the Density Matrix Using the Density Equation: Potential Energy Curves of HF, CH_4, BH_3, NH_3 and H_2O," *Chem. Phys. Lett.* 305, 483-488 (1999).

P.E. Curves
BH_3,CH_4,HF
H_2O,NH_3
Geometries
Frequencies
Calculation
Method

82426. Czuchaj, E., F. Rebentrost, H. Stoll and H. Preuss, "Calculation of Ground- and Excited-State Potential Energy Curves for Barium-Rare Gas Complexes in a Pseudopotential Approach," *Theor. Chem. Acc.* 100, 117-123 (1998).

P.E. Curves
BaNe,BaAr
BaKr,BaXe
Low-lying States
Spectral Constants
D_e

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P.E. Curves
BiS
9 Low-lying States
Spectral Constants
Lifetimes
Calculations

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P.E. Curves
CF,CF^+
Low-lying States
$2^2\Sigma^+$,D,B,A
Lifetimes
Predissociations

(82300) P.E. Surface, Isomerization, Calculations

CH_2I_2

(82301) P.E. Surface, Isomerizations, Isomers, Channels, ΔH_f (CH_2NO,NH_2CO), Calculations

CH_2NO

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P.E. Surface
HCHO
Stationary Points

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(81856) P.E. Surface, Channels, Products — $C_2H_3^+ + C_2H_6$

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(81876)	P.E. Surfaces, Channels, Energies	$Ne^+(^2P)+H_2$
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NeH,ArH
KrH,XeH
Ground States
Well Depths
r_e

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P.E. Curves
Ne_2,Ar_2
Kr_2,Xe_2
Low-lying States
Long Range

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P.E. Surface
O_3
Optimization
Level Fitting

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P.E. Surfaces
$O_3(1^1A',2^1A')$
Conical
Intersection
Seam

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P.E. Curves
PCl(X)
Spectral Constants
D_0
Calculations

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P.E. Curves
Rb_2(b,A)
Long Range
Vibrational Levels
Perturbations
Calculations

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P.E. Curves
RgXe
(Rg=Kr,Ar,Ne)
Irregularities
Explanation

82453. Ornellas, F.R., and A.C. Borin, "The Hidden Facet of the $C^3\Pi$ State of SO," *Mol. Phys.* 94, 139-145 (1998).

P.E. Curves
$SO(C^3\Pi,C'^3\Pi)$
Spectral Constants
T_e,r_e

82454. Nachtigall, P., J. Hrusak, O. Bludsky and S. Iwata, "Investigation of the Potential Energy Surfaces for the Ground X^1A_1 and Excited C^1B_2 Electronic States of SO_2," *Chem. Phys. Lett.* 303, 441-446 (1999).

P.E. Surfaces
SO_2(C,X)
Predissociation
Stationary Points
Double Minimum Potential

82455. Heinemann, C., W. Koch and P.-O. Widmark, "The Tellurium Dimer and Its Anion," *Mol. Phys.* 92, 463-470 (1997).

P.E. Curves
Te_2, Te_2^-
Low-lying States
Spectral Constants
D_0, EA, Energies

82456. Wang, Y., and M. Dolg, "Pseudopotential Study of the Ground and Excited States of Yb_2," *Theor. Chem. Acc.* 100, 124-133 (1998).

P.E. Curves
Yb_2
Low-lying States
Spectral Constants
D_e, IP

44. ATOMIC/MOLECULAR STRUCTURES

(See also Section 26 for Spectrally Measured Structures)

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Structural Calculations
$AlOH^+$, $HAlO^+$
Isomerization Barrier
v,J Levels
AlO^+
Electronic Structure

82458. Ghanty, T.K., and E.R. Davidson, "Reassignment of the $AlSi^-$ Photoelectron Spectrum by ab Initio Configuration Interaction Calculations," *Mol. Phys.* 96, 735-740 (1999).

Structural Calculations
AlSi, $AlSi^-$
Low-lying States
Photoelectron Spectral Assignments

82459. Wesendrup, R., J.K. Laerdahl and P. Schwerdtfeger, "Relativistic Effects in Gold Chemistry. VI. Coupled Cluster Calculations for the Isoelectronic Series $AuPt^-$, Au_2 and $AuHg^+$," *J. Chem. Phys.* 110, 9457-9462 (1999).

Structural Calculations
$AuHg^+$, Au_2
$AuPt^-$
Spectral Constants
D_e, IP

(82521) n = 1-3, ΔH_f, Geometries, Frequencies, Structural Calculations

BF_n, BF_n^+
BCl_n, BCl_n^+

82460. Hinze, J., O. Friedrich and A. Sundermann, "A Study of Some Unusual Hydrides: BeH_2, BeH_6^+ and SH_6," *Mol. Phys.* 96, 711-718 (1999).

Structural Calculations
BeH_2, SH_6
BeH_6^+
Geometries
Stabilities

82461. Schautz, F., H.-J. Flad and M. Dolg, "Quantum Monte Carlo Study of Be_2 and Group 12 Dimers M_2 (M=Zn,Cd,Hg)," *Theor. Chem. Acc.* 99, 231-240 (1998).

Structural Calculations
Be_2, Cd_2
Hg_2, Zn_2
Spectral Constants
D_e

82462. Koput, J., "Ab Initio Study on the Equilibrium Structure and XCN Bending Energy Levels of Halofulminates: BrCNO," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 6017-6022 (1999).

Structural Calculations
BrCNO
Geometries
Bending Frequencies

82463. Xiao, H., Z. Chen and X. Gong, "Theoretical Study on Tetrazole and Its Derivatives. I. Ab Initio Study on Chlorotetrazole," *Chinese Sci. Bull.* 43, 480-483 (1998).

Structural Calculations
c-CHN_4Cl
4 Isomers
Geometries
Energies

82464. Shim, J.-Y., and J.P. Bowen, "Molecular Mechanics Studies of Acyl Halides. I. Molecular Structures and Conformational Analysis. II. Vibrational Spectra," *J. Computat. Chem.* 19, 1370-1386, 1387-1401 (1998).

Structural Calculations
C(H)OX, CH_3COX
C_2H_5COX, C_3H_7COF
C_3H_7COCl
Geometries
Frequencies
X=F,Cl,Br,I

82465. Bruna, P.J., M.R.J. Hachey and F. Grein, "The Electronic Structure of the H_2CO^+ Radical and Higher Rydberg States of H_2CO," *Mol. Phys.* 94, 917-928 (1998).

Structural Calculations
CH_2O^+(1^2A_1, 1^2B_1, X)
CH_2O Rydberg State Energies
Geometries
Frequencies

82466. Mladenovic, M., P. Botschwina, P. Sebald and S. Carter, "A Theoretical Study of the Acetylide Anion, HCC^-," *Theor. Chem. Acc.* 100, 134-146 (1998).

Structural Calculations
C_2H^-
Geometry
Frequencies
Transition Moment

82467.	El Youssoufi, Y., M. Herman and J. Lievin, "The Ground Electronic State of 1,2-Dichloroethane. I. Ab Initio Investigation of the Geometrical, Vibrational and Torsional Structure," *Mol. Phys.* 94, 461-472 (1998).	Structural Calculations $C_2H_4Cl_2$ Geometry Frequencies
82468.	Ma, N.L., and M.W. Wong, "Ethenedithione, S=C=C=S; Does It Obey Hund's Rule?," *Angew. Chem. Int. Ed. Engl.* 37, 3402-3404 (1998).	Structural Calculations C_2S_2 Low-lying States Geometry Frequencies ΔH_f ,D,IP,EA
(82533)	Structural Calculations, ΔH_f , S, Cp, Geometries, Frequencies, Calculations	8 Fluorinated Propanes
82469.	Stanton, J.F., and K.S. Byun, "Coupled-Cluster Studies of Singlet Propynylidene," *Mol. Phys.* 96, 505-509 (1999).	Structural Calculations C_3H_2 Geometry Automerization
82470.	Miyoshi, E., and N. Shida, "An ab Initio Study on the Structure of the Ground State of the C_3O_2 Molecule," *Chem. Phys. Lett.* 303, 50-56 (1999).	Structural Calculations C_3O_2 Geometry Frequencies
82471.	Giuffreda, M.G., M.S. Deleuze and J.-P. Francois, "Structural, Rotational, Vibrational and Electronic Properties and Ionized Carbon Clusters C_n^+(n=4-19)," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 5137-5151 (1999).	Structural Calculations C_n^+,n=4-19 Geometries Frequencies IR Spectra
82472.	Blanksby, S.J., S. Dua and J.H. Bowie, "Generation of Two Isomers of C_5H from the Corresponding Anions: A Theoretically Motivated Mass Spectrometric Study," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 5161-5170 (1999).	Structural Calculations C_5H,C_5H^- Isomers Stabilities C_2CHC_2 Observation
82473.	Grossman, J.C., W.A. Lester Jr and S.G. Louie, "Cyclopentadiene Stability: Quantum Monte Carlo, Coupled Cluster, and Density Functional Theory Determinations," *Mol. Phys.* 96, 629-632 (1999).	Structural Calculations *c*-C_5H_6 Stability
(82309)	Product Structures, Unimolecular Dissociation, $C_{10}H_8^+$, C_2H_2 Loss, Measurements	$C_8H_6^+$

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Structural Calculations
CaO_2, ScO_2
TiO_2
Low-lying States
Geometries
Frequencies

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Structural Calculations
FCN,ClCN
FCN^+(A,X)
$ClCN^+$(A,X)
IPS
Photoelectron Spectral Simulation

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Structural Calculations
F_2, F_2^+, F_2^-
SF, SF^+, SF^-
Geometries
Frequencies

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Structural Calculations
FeO_n, FeO_n^-
$n=1$-4
Geometries
Low-lying States
D_0, EA

82478. Cao, Z., M. Duran and M. Sola, "Low-lying Electronic States and Molecular Structure of Fe_2O_2," *J. Chem. Soc., Faraday Trans.* 94, 2877-2881 (1998).

Structural Calculations
Fe_2O_2
Geometries
Low-lying States
IR Frequencies

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Structural Calculations
HF,DF,TF
Spectral Constants
IR Spectrum Calculations

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HOCl
Vibrational Assignments
Calculation Method

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Structural
Calculations
cis-trans-HONO
Frequencies

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Structural
Calculations
HO_2^+
Low-lying States
P.E. Surfaces
Geometries
Energies

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Structural
Calculations
LiB,LiB^+
Low-lying States
Spectral Constants
D_0

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Structural
Calculations
LiCNO,LiNCO
NaCNO,NaNCO
Geometries
Relative
Stabilities

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Structure
LiCCH,NaCCH
KCCH
Millimeter Spectra

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Structural
Calculations
$NO^+.N_2$
Geometry
ΔH_f

82487. Martin, J.M.L., and P.R. Taylor, "Benchmark ab Initio Thermochemistry of the Isomers of Diimide, N_2H_2, Using Accurate Computed Structures and Anharmonic Force Fields," *Mol. Phys.* 96, 681-692 (1999).
Structural
Calculations
N_2H_2
Isomers
Geometries
Frequencies
ΔH_f

82488. McCarthy, M.C., J.W.R. Allington and K.O. Sullivan, "A Quadratic Configuration Interaction Study of N_2O and N_2O^-," *Mol. Phys.* 96, 1735-1737 (1999).
Structural
Calculations
N_2O,N_2O^-
Geometries
Frequencies
EA

82489. Soldan, P., E.P.F. Lee and T.G. Wright, "Interaction Energies of the $Na^+.Rg$ Complexes (Rg=He,Ne and Ar): Basis Set Considerations for Na^+," *J. Chem. Soc., Faraday Trans.* 94, 3307-3312 (1998).

Structural Calculations
Na^+He, Na^+Ne
Na^+Ar
r_e, D_e

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Structural Calculations
21 Sulfur Containing Molecules
Geometries
Frequencies
Method Comparisons

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Structural Calculations
$Si(CH_2)H_2$
Geometries
Frequencies

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Structural Calculations
$SiCl_2$(a,A,X)
Geometries
Frequencies
Energies
Emission Spectra

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Structural Calculations
FSiO, ClSiO
BrSiO, F_2SiO
Cl_2SiO, Br_2SiO
Geometries
Frequencies
D_e

82494. Boldyrev, A.I., and J. Simons, "Ab Initio Study of the Bonding of Zinc Atoms to First- and Second-Row Main Group Atoms," *Mol. Phys.* 92, 365-379 (1997).

Structural Calculations
ZnM
M=Li through Ar
Geometries
Frequencies
D_0

45. ENERGY TRANSFER

(See also Section 27 for Electronically Excited State Relaxation Processes)

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82496.	Parks, H.V., E.M. Spain, J.E. Smedley and S.R. Leone, "Experimental Investigation of the Initial-State Alignment Dependence in the Energy Pooling Process: $Ca(4s4p^3P_1)+Ca(4s4p^3P_1)\rightarrow Ca(4s4p^1P_1)+Ca(4s^2)$," *Phys. Rev. A: At. Mol. Opt. Phys.* 58, 2136-2147 (1998).	E-E Pooling $Ca(^3P_1)+Ca(^3P_1)$ $(^1P_1)$ Product Cross Sections Polarization Effects
(82443)	Nonradiative Lifetimes, Vibrational Energy Levels, P.E. Curve, Calculations	LiH(C)
82497.	Grushevsky, V., M. Jansons and K. Orlovsky, "A Study of Inelastic Collisions Rb(7S)+Rb(5S): Theoretical Aspects," *Phys. Scr.* 56, 245-251 (1997).	E-E Transfer $Rb(7^2S)+Rb$ $Rb(5^2D)$ Product Cross Sections Calculations
82498.	Sibert III, E.L., "A Perturbative Treatment of Classical Vibrational-Translational Energy Transfer in Colinear Collisions of an Atom and a Diatomic Molecule," *Chem. Phys. Lett.* 307, 437-444 (1999).	V-T Transfer A+BC Average Energy Transfers General Theory
(82216)	Rate Constants, Temperature Dependences, Vibrational Effects	$CH(v=1,0)+H_2O,D_2O$ $CD(v=2,1,0)+H_2O,D_2O$
82499.	Quack, M., and M. Willeke, "Ab Initio Calculations for the Anharmonic Vibrational Resonance Dynamics in the Overtone Spectra of the Coupled OH and CH Chromophores in CD_2H-OH," *J. Chem. Phys.* 110, 11958-11970 (1999).	IVR CHD_2OH Frequency Coupled Modes Calculations
82500.	Boyarkin, O.V., T.R. Rizzo and D.S. Perry, "Intramolecular Energy Transfer in Highly Vibrationally Excited Methanol. II. Multiple time Scales of Energy Redistribution," *J. Chem. Phys.* 110, 11346-11358 (1999).	IVR CH_3OH Overtone Combination Sub ps Energy Flows

82501.	Boyarkin, O.V., T.R. Rizzo and D.S. Perry, "Intramolecular Energy Transfer in Highly Vibrationally Excited Methanol. III. Rotational and Torsional Analysis," *J. Chem. Phys.* 110, 11359-11367 (1999).	IVR $CH_3OH(3,5,6\nu_{OH})$ Spectral Analysis
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$D(ArCl(X,I_{3/2},II_{1/2}))$
$D(ArCl^-)$

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Geometries
Frequencies
Calculations

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(82238)	Isodesmic Reaction Scheme Calculations	$\Delta H_f(FC(O)O_2)$ $\Delta H_f((FCO)_2O_2)$
(82328)	Heats of Reaction, P.E. Surfaces, Reaction Dynamics, Calculations	$CF_2,SiF_2+C_2H_4$ $CH_2,SiH_2+C_2H_4$ $GeF_2,SnF_2+C_2H_4$ $GeH_2,SnH_2+C_2H_4$
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(82332)	Unimolecular Dissociations, Reaction Dynamics, Calculations	ΔH_f,IP,PA $C(SH)_2,HCSSH$
(82336)	P.E. Surface, Channels, HCN Formation, Calculations	$\Delta H_f(CH_3NS)$ Isomers
(82348)	$CH_3SCH_2O_2+M$, Reaction Dynamics, M=9 Reactants, Rate Constants, Calculations	$\Delta H_f(CH_3O_2,CH_3SO)$ $\Delta H_f(CH_3SO_2,CH_3SO_3)$ $\Delta H_f(CH_3SCH_2O)$
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(82347)	Reaction Dynamics, $CH_3SCH_2+O_2$, Energy Barrier	$\Delta H_f(CH_3SCH_2)$
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(82433)	P.E. Curves, CaAr, SrAr($^{1,3}\Sigma$,$^{1,3}\Pi$,X), Spectral Constants, Calculations	D_e(CaAr,SrAr)
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(82477)	Structural Calculations, Geometries, Low-lying States	D_0,EA(FeO_n) n=1-4
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(82053)	Photoassociative RE2PI Spectrum, Constants	$D_e(K_2(1_u))$
(82483)	Structural Calculations, LiB, LiB^+, Low-lying States, Spectral Constants	D_0(LiB)
(82054)	Photodissociation Spectra, Constants	$D_0(Mg^+Ne(A,X))$
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(82487)	Structural Calculations, Isomers, Geometries, Frequencies	$\Delta H_f(N_2H_2)$
(82378)	$NS+NH_2$ P.E. Surfaces, Reaction Dynamics, Channels	$\Delta H_f(N_2H_2S)$ Isomers
(82488)	Structural Calculations, Geometries, Frequencies	EA(N_2O)
(82489)	Structural Calculations, r_e	$D_e(Na^+He,Na^+Ne)$ $D_e(Na^+Ar)$
(82446)	P.E. Curves, Ground States, Well Depths, r_e	NeH,ArH KrH,XeH
(82073)	Low-lying Electronic States, Spectral Constants, Calculations	$D_0(NiC)$
(82419)	v,J Energy Levels, v≤25 Bound States, Calculations	$D_0((O_2)_2)$
(82420)	v,J Energy Levels, v=0,0 and 1,0 Dimers, Bound States, Calculations	$D_0((O_2(a))_2)$
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(82456) P.E. Curves, Low-lying States, Spectral Constants — D_e, IP(Yb_2)

(82494) Structural Calculations, M=Li thru Ar, Geometries, Frequencies — D_0(ZnM)

(82089) $^1\Sigma^+$, $^1\Pi$ van der Waal States, LIF Spectra, Constants, Bond Lengths — D_0(ZnNe)

47. EXPERIMENTAL METHODS

(82403) Excited State, Vibrational Cooling, Polyatomics, Theory — Laser Pumping Method

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Orientation
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